

from Fig. 4, the energy loss of the meson on the basis of the present model tends on the average to be slightly less than that for a collision with a free nucleon.

V. CONCLUSIONS

The use of Eq. (16') should provide a direct means of deducing the values of $d\sigma_N/d\Omega$ (that is, the cross section for scattering mesons on free neutrons) from experiments on the scattering by deuterons and protons for momentum transfers large enough that H_2 is small. Comparison of the scattering from deuterium at large and small angles should provide information about the relative phase of waves scattered from neutrons and protons.¹⁷ This phase is described by the factor $\cos\omega$ in Eq. (16'), which may, of course, be a function of the scattering angle.

¹⁷H. A. Bethe and R. R. Wilson, reference 5, have shown that this is of importance in describing the scattering of mesons in complex nuclei.

For these purposes the readily applied closure approximation is satisfactory.

We are indebted to Mr. Richard I. Mitchell, Mr. Glen Culler, Mr. Burns Macdonald, and other members of the computing group at the Radiation Laboratory for performing most of the numerical calculations described in this paper.

This work was performed under the auspices of the Atomic Energy Commission.

Note added in proof:—Since many meson scattering experiments are being done by attenuation methods, it is desirable to know the cross section for charge exchange scattering. This can be calculated simply from the theory above, using the closure approximation. If we let $d\sigma_p^{\text{exch}}/d\Omega$ be the exchange cross section for π^- on protons, we obtain for the exchange cross section for π^- on deuterons:

$$\frac{d\sigma_{\pi^-D}^{\text{exch}}}{d\Omega} = \frac{d\sigma_p^{\text{exch}}}{d\Omega} [1 - fH_2],$$

where H_2 is given by Eq. (17) and f is a fraction depending upon the amount of spin flip.

Term Values in the 3d⁵4s Configuration of Fe III

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(Received August 8, 1951)

The theoretical formulas for d^5s are compared with the experimental data of Fe III. The mean deviation between theory and experiment is found to be $\pm 852 \text{ cm}^{-1}$.

We compared the values of the parameters B and G_2 which are required to give correctly the observed separations between certain pairs of terms. Adding to the theory a correction term proportional to $L(L+1)$ leads to consistent values of all the radial integral parameters. The mean deviation between the theory corrected in this manner and experiment is reduced to 105 cm^{-1} .

I. INTRODUCTION

IN conjunction with the results of two previous papers,^{1,2} this study completes the analysis of the term values of the 3d⁵4s and 3d⁶ configurations in Fe III and Mn II.

A second purpose of this study is to show that the errors between theory and experiment are simply related to the orbital quantum number. Since 23* of the 32 possible terms of the 3d⁵4s configuration of Fe III are known, there is a large amount of experimental data to verify this conclusion. In addition, the term values are not appreciably affected by interactions with nearby configurations, so that the relationship of the errors to the orbital quantum number represents a polarization effect. If this effect is assumed similar in the same configurations of different atoms, one can

predict more accurately the positions of terms for the experimentalist. We have tentatively made such an application of the results of this paper in a previous paper and have also used the results to verify the experimental assignments of terms to their configurations.²

II. TERM VALUES

The experimental term values are taken from Edlen and Swing.³ The theoretical formulas are the same as those used for d^5s in our previous calculations² for Mn II, and the parameters were evaluated by least squares. The results of the calculation are given in column one of Table I; the mean deviation between theory and experiment is 852 cm^{-1} .

The theoretical formulas for all terms observed in 3d⁵4s of Fe III are rational with the exception of the two terms based on the ²D parent. Partly as a matter of convenience, these two terms were not included in the calculation. However, our subsequent results (Table II) will indicate that the (²D)¹D term observed at

¹R. E. Trees, Phys. Rev. **82**, 683 (1951).

²R. E. Trees, Phys. Rev. **83**, 756 (1951).

* *Note added in proof:*—There are 26 known term values; the 3 highest levels were inadvertently overlooked. The values for these levels are included in Table I. The failure to include them in the least squares calculation has no effect on the conclusions.

³B. Edlen and P. Swings, Astrophys. J. **95**, 532 (1942).

TABLE I. Term values of the $3d^4s$ configuration of Fe III (cm^{-1}). (1) No correction; (2) With $L(L+1)$ -correction.

Term	Obs.	(1)		(2)	
		Calc.	Diff.	Calc.	Diff.
$(^6S)^7S$	30088	30159	71	29991	-97
$(^6S)^5S$	40999	41143	144	40887	-112
$(^4G)^5G$	63465	62822	-643	63512	47
$(^4P)^5P$	66509	67948	1439	66686	177
$(^4D)^5D$	69776	70030	254	69791	15
$(^4G)^3G$	70713	70145	-568	70776	63
$(^4P)^3P$	73790	75270	1480	73951	161
$(^4D)^3D$	77028	77353	325	77054	26
$(^2I)^3I$	79847	78004	-1843	79867	20
$(^2D)^3D$	82413	(84167)	(1754)	(82855)	(442)
$(^4F)^5F$	83238	83393	155	83370	132
$(^2I)^1I$	83429	81666	-1763	83499	70
$(^2F)^3F$	84380	85189	809	84189	-191
$(^2D)^1D$	86846	(87829)	(983)	(86487)	(-359)
$(^2F)^1F$	87901	88850	949	87821	-80
$(^2H)^3H$	88775	88278	-497	88818	43
$(^2G)^3G$	89811	89330	-481	89733	78
$(^4F)^3F$	90464	90715	251	90633	169
$(^2H)^1H$	92523	91939	-584	92450	-73
$(^2F')^3F$	93395	93449	54	93320	-75
$(^2G)^1G$	93512	92992	-520	93365	-147
$(^2F')^1F$	97040	97110	+70	96952	-88
$(^2S)^3S$		99627		98701	
$(^2S)^1S$		103288		102333	
$(^2D')^3D$	105914	106812	898	105930	16
$(^2D')^1D$	109570	110473	903	109562	-8
$(^2G')^3G$	114336	114019	-317	114469	133
$(^2G')^1G$	117950	117681	-269	118101	151
$(^2P)^3P$		131524		131008	
$(^2P)^1P$		135185		134640	
$(^2D'')^3D$		139729		138924	
$(^2D'')^1D$		143389		142556	
A		75350.75		76113.95	
B		1029.66		1058.36	
C		4107.18		3901.33	
G_2		1830.70		1816.00	
				80.74	
Mean deviation			852 cm^{-1}		105 cm^{-1}

86,846 cm^{-1} may be disturbed by configuration interaction with the $^1D'$ term of the $3d^6$ configuration which is not known experimentally but which we have predicted at 76,137 cm^{-1} .¹ Interactions with other terms of the $3d^6$ configuration should produce negligible effects (i.e., less than 100 cm^{-1}), since the interacting terms are 45,000 cm^{-1} or more apart in all cases. It is likely that interactions with the $3d^4s^2$ configuration are also small, but since no terms of this configuration are known experimentally we cannot be sure that this is so.

III. CONSISTENCY OF THE PARAMETER G_2

It has been pointed out⁴ that the errors between theory and experiment in fitting the $3d^4s$ configuration of VI are similar in magnitude and sign to the errors in fitting the $3d^4$ parent term in VII. The fact that the error is mainly in the parent term seems generally true, and has been pointed out in connection with the comparison of $3d^24p$ of Ti II and the $3d^2$ parent term in Ti III.⁵ The addition of a 4s electron to the $3d^5$ parent

introduces an additional parameter G_2 into the calculations. We conclude that this parameter must be definable with an accuracy that is better than the over-all accuracy of the theory, i.e., the mean deviation of our result, as the error of the parent term would otherwise not dominate.

We have checked this conclusion by subtracting the experimental values for the two possible terms that result when the 4s electron is added to the $3d^5$ parent. The results are given in Table II. We see that the separations of the two terms based on the 6S and of the four pairs of terms based on the quartets of d^5 lead to G_2 values that are included in the limits $G_2=1813\pm 7$. As was already pointed out, the separation of terms based on the 2D may be in error owing to interaction with the d^6 configuration. Even excluding this value, however, the G_2 values are much less consistent for terms based on doublet parents, being included in the limits $G_2=1815\pm 59$. We find that the mean deviation in explaining the ten separations of terms based on the same parents with a single parameter $G_2=1815 \text{ cm}^{-1}$ will be about 55 cm^{-1} , which is consistent with the conclusion that the errors are determined chiefly by the parent term.

Part of the inconsistency in G_2 values is due to neglect of nondiagonal spin orbit effects. Our calculation of these effects in the d^6 configuration of Fe III shows that the mean square value of the level shift is about 45 cm^{-1} . We have already pointed out that the effects of configuration interaction are small, but these effects would not be negligible in this calculation, and they would also require consideration. In view of our neglect of these effects, we cannot determine more exactly how consistently the value of the parameter G_2 is defined by subtracting terms based on the same parent; it also seems likely that the close agreement of G_2 values for term based on the sextet and quartet parents is partly accidental.

TABLE II. Consistency of G_2 from subtraction of terms based on the same parent.

Parent	Separation	G_2
6S	10911	1818
4G	7248	1812
4P	7281	1820
4D	7252	1813
4F	7226	1806
2I	3582	1791
2D	(4433)	(2216)
2F	3521	1760
2H	3748	1874
2G	3701	1850
$^2F'$	3645	1822
Limiting values of		G_2
Sextet parent		1818
Quartet parents		1813 \pm 7
Doublet parents		1815 \pm 59

⁴ A. A. Schweizer, Phys. Rev. **80**, 1080 (1950).

⁵ G. Racah, Phys. Rev. **62**, 438 (1942).

IV. THE DIFFERENCES BETWEEN THEORY AND EXPERIMENT

Inspection of column 1 of Table I will show that the differences are positive for *S*, *P*, *D*, and *F* terms and are negative for *G*, *H*, and *I* terms. This same conclusion holds for the *d*⁵*s* configuration² in Mn II. We note a general tendency in *d*^{*n*}, *d*^{*n*}*s*, and *d*^{*n*}*s*² configurations for the difference to decrease as the orbital quantum number increases.^{1,4,6} The fact that in *d*² and *d*³ the ³*P* and ¹*D* differences are positive and the ³*F* and ¹*G* differences are negative has been pointed out by Racah.⁵

Consideration of polarization effects would lead one to expect a dependence on spin, which is here not evident; it is hard to see a reason for the dependence on orbital quantum number.⁷ This dependence of the errors on *L* may be considered not adequately demonstrated by the qualitative considerations of the previous paragraph, but the fact that we can find a simple formula for the *L* dependence of the errors that accounts quantitatively for the major part of the errors in the *d*⁵*s* configuration of Fe III is a more convincing demonstration. The use of least squares in evaluating our parameters leads to a difference between the observed and calculated values that is not a very clear indication of the error in the theory which we are using, as the parameters are able to adjust themselves to compensate for the polarization effects. We propose showing that a somewhat different choice of parameters will not greatly increase the mean deviation, but that with this choice the errors will show a regular dependence on the orbital quantum number.

We simplify our considerations by making subtractions which cancel all parameters in the theory except *B*. Six differences were determined in this way, and the comparison with theory is given in Table III. With the least squares value of *B*=1000 cm⁻¹, the mean deviation in explaining these differences is ±1100 cm⁻¹. The average value of these six determinations of *B* is 1039, but the values range from 896 to 1465.

Most of the inconsistency in the values of this parameter can be removed by adding to each theoretical formula a quantity

$$\Delta E = \alpha L(L+1).$$

⁶ A. Many, Phys. Rev. **70**, 511 (1946).

⁷ E. Wigner, Phys. Rev. **46**, 1002 (1934).

TABLE III. Consistency of *B* from subtraction of terms that cancel other parameters (cm⁻¹). (1) No correction; (2) With *L(L+1)*-correction.

Term diff.	Theory	Obs.	(1)		(2)	
			Calc.	Diff.	Calc.	Diff.
(⁴ <i>D</i>) ⁴ <i>D</i> - (⁴ <i>G</i>) ⁴ <i>G</i>	7 <i>B</i> - 14α	6311	7000	689	6172	-139
(⁴ <i>F</i>) ⁴ <i>F</i> - (⁴ <i>P</i>) ⁴ <i>P</i>	15 <i>B</i> + 10α	16729	15000	-1729	16680	-49
(² <i>G</i>) ² <i>G</i> - (² <i>I</i>) ² <i>I</i>	11 <i>B</i> - 22α	9964	11000	1036	9856	-108
(² <i>H</i>) ² <i>H</i> - (² <i>F</i>) ² <i>F</i>	3 <i>B</i> + 18α	4395	3000	-1395	4632	237
(² <i>F</i>) ² <i>F</i> - (² <i>G</i>) ² <i>G</i>	4 <i>B</i> - 8α	3584	4000	416	3584	0
(² <i>D</i>) ² <i>D</i> - (² <i>H</i>) ² <i>H</i>	18 <i>B</i> - 24α	17139	18000	861	17100	-39
			<i>B</i>	1000	1058	
			α	...	81	
			Mean deviation	±1100 cm ⁻¹	±123 cm ⁻¹	

We then find that the six differences of Table III lead to values *B*=1058 and α=81, and the mean deviation in explaining the differences is reduced to ±123 cm⁻¹. Using the known values of *B*, α, and *G*₂, a few more subtractions can be made to show that this correction also gives consistent values for the parameters *C* and *A*.

We have also carried out a least squares calculation after adding this correction to the theory. The results of this calculation are given in column 2 of Table I; the mean deviation between theory and experiment is reduced to ±105 cm⁻¹. Since this is only slightly larger than the deviation that we would expect from neglect of configuration interaction and nondiagonal spin orbit interaction, we conclude that the correction accounts rather fully for the difference between theory and experiment. The mean deviation to which this correction corresponds will be

$$\Delta = \pm \alpha \{ \langle L(L+1) \rangle - \langle L(L+1) \rangle_{\text{av}} \}^2 \}_{\text{av}}^{\frac{1}{2}},$$

where the averages are taken over the experimentally observed terms. For our calculation, this expression has a value ±980 cm⁻¹. As would have to be the case, this is not quite as good an over-all agreement as is indicated by the deviation ±852 cm⁻¹ in column 1 of Table I. However, the difference is not very great, so that our formula for the error

$$\text{Diff} = 1200 - 81L(L+1) \pm 105,$$

when the parameters of column 2 are used, will represent rather closely the trend of the errors when the parameters are evaluated by least squares, as was done in column 1.

I am very grateful to Dr. C. W. Ufford for his continued encouragement and for many helpful discussions.