PHYSICAL REVIEW LETTERS

VOLUME 24 2 MARCH 1970 NUMBER 9

HYPERFINE STRUCTURE IN THE 2^2P STATE OF ATOMIC LITHIUM

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(Received 26 November 1969)

Calculations by two different theoretical methods are in good agreement with each other and with available experimental data on hyperfine splitting and Zeeman level crossing of 2^2P lithium. These results show unequivocally that the contact, spin-dipolar, and orbital hyperfine interactions must be described by three independent parameters.

A nuclear magnetic moment $\vec{\mu}_N$ interacts with atomic electrons through three interaction operators of different spherical tensor symmetry:

$$H_c = \vec{C}\cdot(8\pi g_e/3)\textstyle\sum_i \vec{s}_i\delta(\vec{r}_i),$$
$$H_{\rm dip} = \vec{C}\cdot g_e\textstyle\sum_i[3(\vec{s}_i\cdot\vec{r}_i)\vec{r}_i - r_i^2\vec{s}_i]r_i^{-5},$$
$$H_{\rm orb} = \vec{C}\cdot 2\textstyle\sum_i \vec{l}_i r_i^{-3}, \quad (1)$$

where

$$\vec{C} = (\mu_B\mu_N/Ia_0^3)\vec{I}. \quad (2)$$

Here $g_e = 2.002\,32$, μ_B is the Bohr magneton, and a_0 is the first Bohr radius in hydrogen. The operators in Eq. (1) represent, respectively, the Fermi contact, spin-dipolar, and orbital magnetic hyperfine structure interactions. These operators are each affected differently by terms in the electronic wave function that represent correlation corrections to the traditional Hartree-Fock approximation. They can be characterized by three parameters, respectively a_c, $a_{\rm dip}$, and $a_{\rm orb}$, which give the contribution of each interaction operator to the hyperfine constant a_J in a state with $M_L = L$, $M_S = S$, $M_J = J = L + S$, for the Li^7 isotope.

Calculations of these three parameters have been carried out for the 2^2P excited state of atomic lithium, using a generalization of Brueckner's theory[1] expressed in terms of appropriately defined one- and two-electron Bethe-Goldstone equations.[2] The procedure used in earlier hyperfine-structure calculations by this method[3] has been modified so that all virtual excitations refer to complete configurations rather than just to single Slater determinants. In this form, the calculations are equivalent to a method used by Schaefer and Harris,[4] who expressed the Bethe-Goldstone configuration-interaction procedure in terms of $\vec{L}^2$ and $\vec{S}^2$ eigenfunctions. Details of these calculations will be published separately.[5] Computed values of the three basic hyperfine parameters are listed in Table I (RKN).

A recent calculation for Li (2^2P) by Lyons, Pu, and Das,[6] using the Brueckner-Goldstone perturbation method developed by Kelly,[7] is also expected to give results of high quantitative accuracy. These results are also listed in Table I (LPD).

Two observable fine-structure level crossings occur in the 2^2P term of Li as a result of Zeeman splitting. The low-field crossing, between $J, M_J = (\frac{3}{2}, -\frac{3}{2})$ and $(\frac{1}{2}, \frac{1}{2})$, occurs for magnetic field H_l approximately 3200 G. The high-field crossing, between $(\frac{3}{2}, -\frac{3}{2})$ and $(\frac{1}{2}, -\frac{1}{2})$, occurs for H_h near 4800 G, and gives an observable anticrossing signal. A detailed analysis of hyperfine structure effects in level crossing has been carried out and will be published separately.[8] Each

Table I. Comparison of level crossing and hyperfine data for 2^2P lithium. Field intervals ΔH are in Gauss; all other data are in MHz.[a]

Isotope	Crossing Field	Datum	LPD[b]	RKN[c]	Experiment
Li^6	H_ℓ	ΔH_1	2.9118	2.9005	
		ΔH_2	2.9213	2.9096	
	H_h	V_1	6.6992	6.8928	V_{av} =
		V_2	6.7063	6.9009	$6.783 \pm .069$[d]
		ΔH	2.8684	2.8812	
Li^7	H_ℓ	ΔH_1	7.6017	7.5748	$7.5416 \pm .0078$[e]
		ΔH_2	7.6504	7.6183	$7.5957 \pm .0070$[e]
		ΔH_3	7.7122	7.6757	$7.6379 \pm .0127$[e]
	H_h	V_1	21.5533	22.1612	
		V_2	25.0263	25.7505	
		V_3	21.7933	22.4397	
		ΔH_1	7.7566	7.7996	
		ΔH_2	7.6110	7.6375	
Li^7		$a_{1/2}$	45.8879	46.0383	$46.17 \pm .35$[f]
		a_c	-9.5788	-9.8880	$-9.806 \pm .116$[g]
		a_{dip}	-1.8964	-1.8694	$-1.908 \pm .034$[g]
		a_{orb}	8.6727	8.7283	$8.641 \pm .037$[g]
		$a_{3/2}$	-2.8025	-3.0291	$-3.073 \pm .126$[g]

[a]Conversion factors from B. N. Taylor, W. H. Parker, and D. N. Langenberg, Rev. Mod. Phys. 41, 375 (1969); nuclear magnetic moments from N. F. Ramsey, Molecular Beams (Oxford Univ., New York, 1956), p. 172.

[b]Ref. 6.

[c]Ref. 5.

[d]Ref. 10. Preliminary results of a new analysis of experimental data reported in Ref. 11.

[e]Ref. 11.

[f]Ref. 12.

[g]Values obtained from Eqs. (3) in the text.

of the hyperfine crossing field intervals ΔH and anticrossing matrix elements V listed in Table I has been computed as a function of a_c, a_{dip}, and a_{orb}, assuming established values of fundamental constants and of the nuclear magnetic moments. The best available values of the nuclear electric quadrupole moments[9] were used, in combination with computed field gradients, but the quadrupole interaction is small and cannot easily be distinguished from the residual errors of the computed and experimental results. Available experimental data are included in the Table.[10-12]

Observed values of the average high-field anticrossing matrix element $V_{av}{}^h$,[10] of the average low-field crossing interval $\Delta H_{av}{}^l$,[11] and of the hyperfine structure constant $a_{1/2}$[12] can be used to determine experimental values of a_c, a_{dip}, and a_{orb}. The required formulas are[8]

$$a_c = (40c_1 + 14c_2 + 15c_3)/69,$$
$$a_{dip} = (-7c_1 + c_2 + 6c_3)/69,$$
$$a_{orb} = (-5c_1 + 4c_2 + c_3)/23, \quad (3)$$

where

$$c_1 = -(\tfrac{2}{3})^{1/2}[g(Li^7)/g(Li^6)]V_{av}{}^h(Li^6),$$
$$c_2 = (11/6)(\partial\Delta/\partial H)\Delta H_{av}{}^l(Li^7),$$
$$c_3 = -a_{1/2}(Li^7), \quad (4)$$

with[11]

$$\partial\Delta/\partial H = 3.054 \text{ MHz/G} \quad (5)$$

and

$$g(\mathrm{Li}^7)/g(\mathrm{Li}^6) = 2.641\,006. \quad (6)$$

The three hyperfine coupling parameters obtained from Eqs. (3), using observed data in Eqs. (4), are listed in Table I, together with the implied value of $a_{3/2}$. These numbers differ from either set of computed values by roughly 2%. The two sets of computed results, obtained by very different methods, are in substantial agreement with each other and with experiment. The Bethe-Goldstone results (RKN) are within a fraction of 1% of the best established experimental data ($a_{1/2}$ and ΔH for the Li^7 low-field level crossing). The small discrepancy between this calculation and the hyperfine parameters deduced from experimental data is almost entirely due to the difference between computed and observed values of $V_{av}{}^{h}(\mathrm{Li}^6)$. The computed data in Table I should provide useful predictions of those quantities not yet determined experimentally.

The two independent computations, and available experimental data, indicate unequivocally that a_c, a_{dip}, and a_{orb} must be treated as independent parameters. The practice of assuming a fixed relationship among these parameters, obtained from one-electron models, cannot be justified in the analysis of accurate experimental data.

We are indebted to Professor T. G. Eck for a number of valuable discussions, and for allowing use of his recent data prior to publication.

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$H^+ + H^-$ MUTUAL NEUTRALIZATION CROSS SECTION OBTAINED WITH SUPERIMPOSED BEAMS*

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The ion-ion mutual neutralization cross section for $H^+ + H^-$ has been measured over the barycentric energy range from 0.15 to 300 eV using a merged-beam technique. The results are compared with theoretical calculations and with a recent higher energy experimental measurement. An estimate of the thermal rate coefficient is made.

The ion-ion mutual neutralization cross section has been measured for $H^+ + H^-$ using a superimposed beam technique. The barycentric energy range of the measurements is 0.15 to 300 eV. This is the first measurement of this important cross section at energies below 125 eV. The data compare very favorably with the results of Rundel, Aitken, and Harrison,[1] who used beams intersecting at 20°, in the region of overlap. There has been substantial theoretical interest in ion-ion mutual neutralization,[2-5] and especially in the $H^+ + H^-$ reaction.[2-4] This system is well suited for an experimental test of theoretical calculations because of its simplicity and of the fact that the initial states are well defined.

The technique, which has been described in detail elsewhere,[6] involves merging the positive and negative ion beams of different speeds by magnetic deflection, and observing their interaction over a known path length (see Fig. 1). Both beams have laboratory energies E^+ and E^- in the keV range, but can have relative energies W as low as 0.15 eV while in the interaction region.

After traversing the 30-cm interaction length