

and  $l$  are in the FR.

By taking a derivative<sup>2</sup> of the expression (8a) for  $\text{Re} \ln(\Lambda_e/\Lambda_0)$ , we obtain (for  $\mu \leq \pi/2$ ) the energy difference  $\Delta E$  between the first excited states and ground state as a function of  $\alpha_1$  and  $\alpha_2$ . Baxter<sup>2</sup> has shown that the transfer matrix  $T(\alpha_b = \lambda)$  is equal to  $2^N$  times the cyclic shift operator that moves all spins one site to the left. Therefore, from  $\text{Im} \ln(\Lambda_e/\Lambda_0)$ , calculated at  $\alpha_b = \lambda$ , one can extract the momentum difference  $\Delta P$  between the excited states and the ground state in terms of  $\alpha_1$  and  $\alpha_2$ . We define two new variables  $q_1$  and  $q_2$  by

$$q_i = \int_{-K_m}^{K_m} m^{\alpha_i/\pi} \text{dn}(\varphi, m) d\varphi.$$

Then

$$\Delta P = q_1 + q_2 - (\omega_1 + \omega_2)\pi - \pi, \quad (11a)$$

$$\Delta E = -J_z \text{sn}(2\xi, l) K_m (K_1')^{-1} \times [(1 - m^2 \cos^2 q_1)^{1/2} + (1 - m^2 \cos^2 q_2)^{1/2}], \quad (11b)$$

where  $m$  is determined from  $K_m'/K_m = \lambda/\pi$ . The range of the  $q_i$  is  $0 \leq q_i \leq \pi$ . For a given value of  $q_1$  and  $q_2$ , there are eight states, and the statistics of the excitations is believed to be of the Fermi-Dirac type.

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<sup>8</sup>We wish to remark that the whole integral equation formalism suffers from ambiguities in that the branches of the logarithms appearing in the formalism are not *a priori* specified. We have chosen these branches such that the known results in the decoupling ( $\mu \rightarrow \pi/2$ ) and ice limits are recovered and the excitation energies of the  $X$ - $Y$ - $Z$  model are correct in the  $X$ - $Y$  and Heisenberg-Ising limits.

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## Quadrupole Moment of the Deuteron\*

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The electric field gradient in the HD and D<sub>2</sub> molecules has been calculated from 87-term wave functions of the James and Coolidge type. With the use of experimental values of the quadrupole interaction constant, the electric quadrupole moment of the deuteron is found to be 0.2875 F<sup>2</sup> which is 2% larger than the most recent values. The estimated error is 0.002 F<sup>2</sup>.

The quadrupole moment of the deuteron,  $Q$ , has long served as a touchstone for models of the nucleon-nucleon interaction because of its connection with the tensor force, without which  $Q$  would vanish. At the present time  $Q$  cannot be directly determined experimentally; it can be extracted from the electric quadrupole interaction constant  $eqQ/h$  with the aid of a theoretically

calculated field gradient  $q$ . However, quantitative calculation of the field gradient<sup>1-5</sup> for such simple molecules has proved difficult. Code and Ramsey<sup>6</sup> cast doubt on the most recent calculation<sup>5</sup> by showing that the results were not consistent with their D<sub>2</sub> ( $J=1$ ) and the earlier<sup>7</sup> HD ( $J=1$ ) interaction constants. Signell and Parker<sup>8</sup> have noted the extent and aspects of the seriousness

of the disagreement among reported values of the quadrupole moment. Our results, obtained from molecular wave functions fully optimized at each internuclear distance and expanded in a basis set 8 times larger than in previous work, appear to have converged and are consistent with the set of three measured interaction constants.<sup>6,7</sup>

The field gradient along the molecular axis evaluated at one of the nuclei is

$$q = 2e \langle q'(R) \rangle_J,$$

with the average being taken over the molecular zero-point vibration in the  $J$ th rotational state and

$$q'(R) = R^{-3} - \int d^3r_1 d^3r_2 \psi^2(\vec{r}_1, \vec{r}_2, R) V''(\vec{r}_1, \vec{r}_2), \quad (1)$$

where  $V''(\vec{r}_1, \vec{r}_2) = P_2(\theta_1)r_1^{-3} + P_2(\theta_2)r_2^{-3}$ ,  $r_i$  is the distance of the  $i$ th electron from the nucleus under consideration,  $\theta_i$  is the angle between  $\vec{r}_i$  and the molecular axis,  $R$  is the internuclear distance, and  $\psi$  is the molecular electronic wave function.

Using the prolate spheroidal coordinates of each electron,  $\xi = (r_a + r_b)/R$  and  $\eta = (r_a - r_b)/R$ , where  $r_a$  and  $r_b$  are distances from nuclei  $a$  and  $b$ , we take the molecular electronic wave function to be

$$\psi = \sum_{m_p r_s \mu} C_{m_p r_s \mu} (\xi_1^m \eta_1^p \xi_2^r \eta_2^s + \xi_1^r \eta_1^s \xi_2^m \eta_2^p) \rho^\mu \times \exp[-\alpha(\xi_1 + \xi_2)], \quad (2)$$

where  $\rho = 2r_{12}/R$ . The parameters  $C_{m_p r_s \mu}$  and  $\alpha$  are, for each  $R$ , determined variationally by minimizing the Rayleigh quotient. From the

work of Kolos and Wolniewicz<sup>9</sup> we chose six terms,  $(m, p, r, s, \mu) = (0, 0, 3, 0, 0)$ ,  $(0, 0, 0, 4, 0)$ ,  $(0, 1, 1, 3, 0)$ ,  $(1, 0, 4, 0, 0)$ ,  $(1, 0, 0, 4, 0)$ , and  $(3, 0, 0, 2, 0)$ , which seemed particularly important in lowering the energy. We were able, in addition, to allow  $(m, p, r, s, \mu)$  to take on the 81 possible combinations of 0, 1, 2, consistent with the symmetry of the  ${}^1\Sigma_g^+$  state. By this means we attempted to avoid omitting components of  $\psi$  relatively more important for  $q$  than the Hamiltonian.

To average over nuclear motion,  $q'(R)$  was calculated at 12 values of  $R$  between 0.95 and 2.1 a.u. The averaging was performed using vibrational wave functions obtained by numerical integration using the adiabatic potential of Kolos and Wolniewicz.<sup>9,10</sup> With 87 terms, for HD( $J=1$ ), D<sub>2</sub>( $J=1$ ), D<sub>2</sub>( $J=2$ ), respectively, we found  $\langle q'(R) \rangle$  to be 0.166 20, 0.166 60, and 0.165 38 a.u. yielding<sup>6,7</sup>  $Q = 0.287 49$ ,  $0.287 45$ , and  $0.287 43$  F<sup>2</sup>. The weighted average is 0.2875(20) F<sup>2</sup>. The error is one half the maximum possible change in  $Q$ , which can be constructed within our 87-term basis, consistent with a change in the energy of  $2.9 \times 10^{-6}$  a.u. (see Table I). It is an estimate, to be discussed elsewhere, of the effect of our truncation of the basis. Other errors are more than 1 order of magnitude smaller. The comparison in Table I includes  $Q$  values calculated with 34 and 66 terms in the basis to verify convergence.

Using our values for  $\langle q'(R) \rangle$  and the experimental  $eqQ/h$  for D<sub>2</sub>( $J=1$ ), "equivalent"<sup>6</sup>  $eqQ/h$  for HD( $J=1$ ) and D<sub>2</sub>( $J=2$ ) are 224.504(30) and 223.396(30) kHz, respectively; corresponding experimental ones are 224.540(60)<sup>7</sup> and 223.380(180).<sup>6</sup>

TABLE I. Values of the quadrupole moment obtained from field-gradient calculations.

Source	Parameters	$D_e$ (a.u.)	$Q$ (F <sup>2</sup> ) <sup>a</sup>
Ref. 1	2	0.149	0.2714 ± 0.0054
Ref. 2	7	0.157	0.2777 ± 0.0056
Ref. 3	6	0.168	0.2738 ± 0.0016
Ref. 5	11	0.173 01	0.2800 ± 0.0005
Ref. 4	10	0.173 76	0.282 ± 0.001
This work	34	0.174 32	0.2898
This work	66	0.174 471 2	0.2874
This work	87	0.174 472 1	0.2875 ± 0.0020
Ref. 10	...	0.174 475 0	...

<sup>a</sup>The first three values of  $Q$  were altered to conform with more recent experimental results. All errors are estimates by the corresponding authors.

We conclude that the  $R$  dependence of our field gradient is in good agreement with experiment.

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## Magnetic Moments of the $7^-$ and $5^-$ ( $\pi h_{9/2}, \nu g_{9/2}$ ) States in $^{210}\text{Bi}$

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The  $g$  factors of the 433-keV  $7^-$  state and the 439-keV  $5^-$  state in  $^{210}\text{Bi}$  which are predominantly ( $\pi h_{9/2}, \nu g_{9/2}$ ) have been measured as  $g(7^-) = 0.302 \pm 0.007$  and  $g(5^-) = 0.306 \pm 0.009$  by a time-differential method using the reaction  $^{208}\text{Pb}(^7\text{Li}, \alpha n)^{210}\text{Bi}$ . From these experimental results, a magnetic moment for the  $g_{9/2}$  neutron of  $\mu = -(1.33 \pm 0.06)\mu_N$  [ $g(\nu g_{9/2}) = -0.296 \pm 0.014$ ] has been deduced. This  $g_{9/2}$ -neutron magnetic moment is in agreement with the Schmidt value corrected for core polarization.

The large anomaly that exists in the magnetic moment of the  $h_{9/2}$  proton single-particle state outside of  $^{208}\text{Pb}$  has represented for some time an important difficulty for nuclear theory. Expected corrections to the magnetic moment for core polarization do not give a satisfactory explanation.<sup>1,2</sup> The high purity of the single-particle states relative to the doubly closed shell of  $^{208}\text{Pb}$  makes the understanding of their magnetic moments essential for the interpretation of nuclear magnetic properties in general. Despite this importance and the  $h_{9/2}$  proton anomaly, there is as yet no experimental information on the magnetic moments of neutron single-particle states outside of  $^{208}\text{Pb}$ . In this context, a measurement of the  $g$  factor of the  $g_{9/2}$  neutron state, which is the lowest neutron single-particle state outside of  $^{208}\text{Pb}$ , is of considerable interest to the basic understanding of this anomalous magnetism. Recently, Nagamiya and Yamazaki<sup>3</sup> have concluded that magnetic moments measured for several proton particle states including the  $h_{9/2}$  state and neutron hole states of the  $^{208}\text{Pb}$  core show evidence for anomalous orbital  $g$  factors.

They suggest an increase in the orbital  $g$  factor for the proton of  $\Delta g_1 = 0.10$  which in turn gives an explanation for the anomalous  $h_{9/2}$  magnetic moment. Their analysis and other more recent work for neutron hole states<sup>4</sup> suggest with less evidence a  $\Delta g_1 \sim -0.05$  for the neutron. The knowledge of the  $g_{9/2}$  single-neutron  $g$  factor would also give an additional check of any  $\Delta g_1$  for the neutron. A theoretical basis for the  $\Delta g_1$  has been discussed in terms of meson exchange currents.<sup>5,6</sup> The low lying levels in  $^{210}\text{Bi}$  have been interpreted<sup>7</sup> as the ( $\pi h_{9/2}, \nu g_{9/2}$ ) negative-parity multiplet with angular momentum  $J$  from 0 to 9 (see Fig. 1). Since the  $g$  factor of the  $h_{9/2}$  proton is known, a measurement of the magnetic moment of a pure member of this multiplet in  $^{210}\text{Bi}$  can yield the  $g_{9/2}$  neutron  $g$  factor. The known  $g$  factor of the  $1^-$  state in  $^{210}\text{Bi}$  fails to give this value, since this specific state has admixtures which make significant contributions to its magnetic moment. The  $7^-$  and  $5^-$  members of this multiplet in  $^{210}\text{Bi}$  are, however, quite pure with negligible magnetic-moment contributions from admixtures. The lifetimes<sup>8</sup> of both of these states are also conve-