QUADRUPOLE MOMENT OF Li^7 AND QUADRUPOLE COUPLING CONSTANT OF Li$_2$[†]

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Recently, the quadrupole coupling constant of Li^7 in LiH has been measured to high accuracy by Klemperer, Gold, and Wharton.[1] When combined with our calculated value of the electric field gradient at the Li^7 nucleus, this measurement leads to a definitive value for the quadrupole moment of Li^7, $Q(\text{Li}^7) = -3.56 \times 10^{-26}$ cm^2. We have also calculated the electric field gradient in Li$_2$. Using $Q(\text{Li}^7)$ calculated from LiH, we find the quadrupole coupling constant for the Li$_2$ molecule to be +0.049 Mc/sec compared with the value of +0.060 Mc/sec estimated by Logan, Coté, and Kusch.[2] This would indicate that the Logan, Coté, and Kusch value may be too large and that it would be desirable for the quadrupole coupling constant of Li$_2$ to be remeasured with higher accuracy in order to check the prediction. The remainder of this Letter presents some details of the molecular calculations.

Our electronic computer calculations of the molecular properties of the LiH and Li$_2$ molecules have been carried out by the Roothaan[3] (Hartree-Fock, self-consistent field, molecular orbital, linear combination of atomic orbitals) procedure as modified by Nesbet.[4,5] Extended sets of basis functions of the Slater type were employed and configuration interaction corrections to the energy and electric field gradient were calculated. For LiH, a basis set of 13 Slater-type orbitals were used, including $p\pi$ functions on both the lithium and hydrogen centers. For Li$_2$, 18 Slater-type orbitals were used (9 on each center), including $p\pi$ functions. In both cases the $p\pi$ functions were found to give large contributions in configuration interaction. For configuration interaction calculations in LiH, the 27 most important configurations are included in the energy and 19 configurations in the electric field gradient. For configuration interaction calculations in Li$_2$, the 28 most important configurations are included in the energy and 24 configurations in the electric field gradient. These calculations were carried out at three internuclear distances, including the internuclear distance corresponding to the minimum energy.

The accuracy to which the molecular wave function has been calculated may be indicated from the following results. For LiH, a total

molecular energy of 99.3 % of the experimental value, and a dissociation energy of 89.3 % of the experimental value were calculated. Similar calculations in Li$_2$ resulted in 99.4 % and 89.9 %, respectively, for these two quantities. The energy of atomic Li, which enters the dissociation energy calculation, was calculated to comparable accuracy (99.4 %).

Recently Klemperer, Gold, and Wharton have measured the quadrupole coupling constant of Li^7 in the LiH molecule[1]; the value $eqQ/h = +346 \pm 2$ kc/sec is found. Our calculated value for the electric field gradient at the Li nucleus is $q/2e = -0.02070 \, a_\text{H}^{-3}$, evaluated at the internuclear distance corresponding to the minimum of the energy. e is the magnitude of the electron charge and a_H is the first Bohr radius. This leads to a value of -3.56×10^{-26} cm^2 for $Q(\text{Li}^7)$, in agreement with predictions from theoretical models of the nucleus.[6] This value is estimated to have an error associated with it of less than 10 %. As distinct from the Li$_2$ case,[7] the electronic and nuclear contributions to the electric field gradient are not nearly equal, the latter being about 0.65 of the former.

For Li$_2$, $q/2e$ is calculated to be $-0.0029 \, a_\text{H}^{-3}$. Together with $Q(\text{Li}^7)$ found above, this leads to a quadrupole coupling constant of +0.049 Mc/sec. The experimental value of Logan, Coté, and Kusch,[2] which is +0.060 Mc/sec, would thus appear to be too large.

A complete account of the molecular calculations will be presented later.

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[2]R. A. Logan, R. E. Coté, and P. Kusch, Phys. Rev. 86, 280 (1952).

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[4]R. K. Nesbet, Quarterly Progress Report, Solid State and Molecular Theory Group, Massachusetts Institute of Technology, October 15, 1955 (unpublished), pp. 4-8.

[5]R. K. Nesbet, Revs. Modern Phys. 32, 272 (1960).

[6]See, for example, S. B. Welles, Phys. Rev. 62, 197 (1942).

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INELASTIC SCATTERING OF 18.9-Mev NUCLEONS FROM THE 9.6-Mev STATE OF C^{12}

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Recently it has been suggested[1] that the 9.6-Mev state of C^{12} has spin and parity $J^{\pi}=3^{-}$ and not 1^{-} as previously supposed.[2] This Letter reports a new analysis of Peelle's[3] 18.9-Mev inelastic proton scattering data, which definitely favors 3^{-} for the 9.6-Mev state. The calculation uses a direct volume interaction with spin-dependent distorted waves.[4]

Peelle's[3] analysis of his data is based upon the direct surface interaction theory, which predicts a $j_K{}^2(kR)$ angular distribution. Using an interaction radius $R=3.3$ fermis, he found a best fit for $K=1$ giving $J^{\pi}=0^{-}$, 1^{-}, or 2^{-}. The same theory applied to inelastic scattering from the 4.4-Mev 2^{+} state of C^{12} gave very poor agreement with experiment.

Levinson and Banerjee[5] showed that the direct-surface-interaction theory is probably inadequate for a nucleus as small as C, and Robson and Robson[4] found spin-orbit effects to be important for 12-Mev nucleons inelastically scattered from the 4.4-Mev level of C^{12}. Thus it was considered essential to take both these effects into account before using Peelle's data to determine the spin and parity of the 9.6-Mev state. In the following, only $J^{\pi}=1^{-}$ or 3^{-} are considered because there exists a reasonable amount of evidence[1] for eliminating other values.

The distorting potential is taken to be the usual Woods-Saxon optical potential plus a Thomas-Fermi spin-orbit potential,[6]

$$V_D(r) = -(V+iW)f(r) + (V_S+iW_S)\left(\frac{\hbar}{m_\pi c}\right)^2 \frac{1}{r}\frac{df}{dr}\,\vec{\sigma}\cdot\vec{L},$$

$$f(r) = \{1 + \exp[(r-R)/a]\}^{-1}. \tag{1}$$

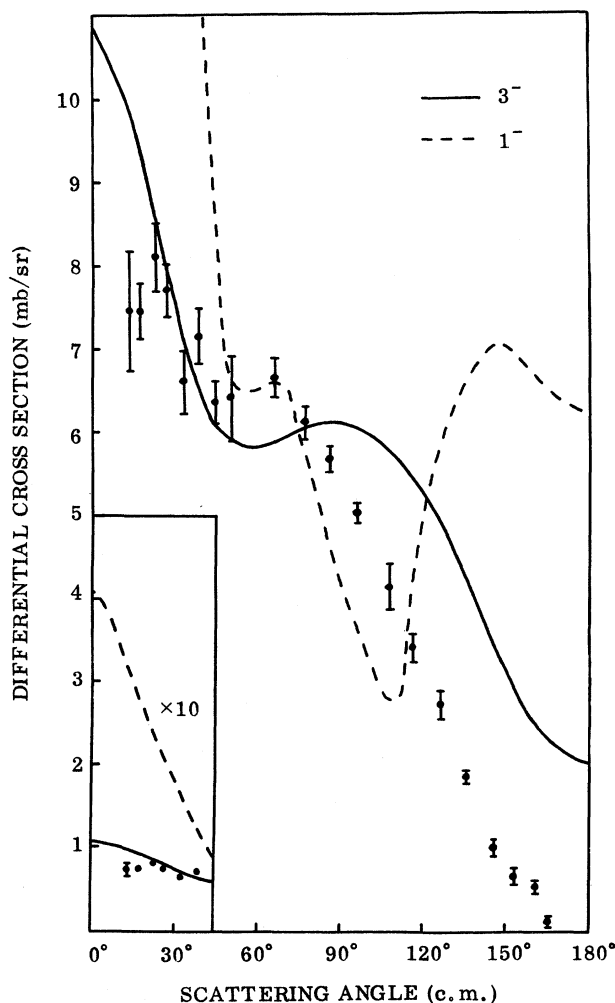The values of V, W, V_S, and W_S used are 45, 12,

FIG. 1. Inelastic nucleon scattering from the 9.6-Mev state of C^{12}. The points are the experimental results of Peelle for 18.9-Mev protons. The theoretical curves are for 18.9-Mev neutrons. The normalization is arbitrary and both curves are fitted at 75°.