226

APPLICATION OF BRUECKNER-GOLDSTONE MANY-BODY PERTURBATION THEORY TO ATOMIC PROPERTIES OF LITHIUM

by

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ABSTRACT OF THE DISSERTATION

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The Brueckner-Goldstone Many-Body Perturbation Theory has been applied to the study of various properties of the lithium atom. These include the hyperfine coupling constant, the correlation energy, the dipole polarizability and shielding factor. The calculation of these atomic properties enables us to test the goodness of the lithium wave function, obtained in this approach, in different regions of the atom. The same set of basis states is used for all four properties, so that the calculation of additional properties requires little extra effort. Associated with this method is the utilization of Feynman-type diagrams, which are interpreted to represent various physical effects such as exchange

polarization, correlation, etc. This in turn facilitates comparisons and evaluations of other methods. The calculation of the hyperfine coupling constant utilizes additional attractive features of this method: the wave function is shown to be an eigenfunction of S^2 to each order of the perturbation; also, formal cancellation of diagrams may be made prior to the calculation. The result, 2.887 a.u., is in close agreement with the experimental value of 2.9096 a.u. The total energy, calculated to be -7.478 a.u., is also in good agreement with the experimental value of -7.47807 a.u. The calculated dipole polarizability is 24.85 Å, while the most recent experimental value is 22±2 Å. An absolute check on the perturbed wave function is provided by the calculation of the dipole shielding factor, whose theoretical value is exactly one. Our calculation yields an excellent result of .958 for this sensitive test. Rapidity of the convergence of the perturbation series is inferred from the fact that accurate results are obtained from the wave function calculated only to the second order.

TABLE OF CONTENTS

TABLE OF CONTENTS (con.)