

226

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

by

Edward Shih-Tou Chang

A dissertation submitted in partial  
satisfaction of the requirements of a  
graduate program in Physics  
for the degree of Doctor of Philosophy

June, 1967

University of California, Riverside

ABSTRACT OF THE DISSERTATION

Application of Brueckner-Goldstone  
Many-Body Perturbation Theory to  
Atomic Properties of Lithium

by

Edward Shih-Tou Chang

Doctor of Philosophy, Graduate Program in Physics

University of California, Riverside, June 1967

Professor Robert T. Pu, Chairman

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  $22 \pm 2$  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

CHAPTER	PAGE
1. Introduction	
a. Critique of previous calculations .....	1
b. Introduction to the Brueckner-Goldstone method .....	6
c. Purpose of dissertation .....	8
d. Survey of succeeding chapters .....	10
2. Formal Brueckner-Goldstone theory	
a. Review of the Brueckner-Goldstone theory .....	12
b. Expectation value of an operator .....	20
3. Application of the BG theory to the Lithium atom	
a. Choice of the single-particle potential .....	24
b. Calculation of the wave function .....	28
c. Eigenfunction of $S^2$ .....	31
4. The hyperfine coupling constant	
a. Discussion of the experimental value .....	35
b. Calculation of normalization diagrams .....	36
c. Calculation of hfs diagrams .....	37
d. Results .....	55
5. The energy	
a. Discussion of the experimental energy .....	59
b. Calculation of energy diagram .....	60
c. Results .....	69
d. Discussion of the wave function in view of the results for the hfs and the energy .....	71

## TABLE OF CONTENTS (con.)

CHAPTER	PAGE
6. Properties in an external electric field	77
a. Definitions and introductory remarks	77
b. The Hartree-Fock perturbation methods	82
c. Analysis of the HF methods in terms of the present theory	87
d. Calculation of the dipole polarizability	94
e. Calculation of the dipole shielding factor	101
f. Summary of results	106
7. Concluding remarks	107
BIBLIOGRAPHY	110
APPENDIX A	114
APPENDIX B	136
APPENDIX C	151
APPENDIX D	156