

AN APPLICATION OF THE LIOUVILLE RESOLVENT METHOD  
TO THE STUDY OF FERMION-BOSON COUPLINGS

by

Barry Lee Bressler

Dissertation submitted to the Faculty of the  
Virginia Polytechnic Institute and State University  
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

in

Physics

APPROVED:

\_\_\_\_\_  
S. P. Bowen, Chairman

✓ \_\_\_\_\_  
L. D. Roper

\_\_\_\_\_  
C. D. Williams

\_\_\_\_\_  
R. K. P. Zia

\_\_\_\_\_  
✓ T. K. Lee

June, 1986

Blacksburg, Virginia

AN APPLICATION OF THE  
LIOUVILLE RESOLVENT METHOD  
TO THE STUDY OF  
FERMION-BOSON COUPLINGS

by

Barry Lee Bressler

Committee Chairman: Samuel P. Bowen  
Physics

(ABSTRACT)

The Liouville resolvent method is an unconventional technique used for finding a Green function for a Hamiltonian. Implementation of the method entails the calculation of commutators of a second-quantized Hamiltonian operator with particular generalized stepping operators that are elements of a Hilbert space and that represent transitions between many-particle states. These commutators produce linear combinations of stepping operators, so the results can be arrayed as matrix elements of the Liouville operator  $\hat{L}$  in the Hilbert space of stepping operators. The resulting  $\hat{L}$  matrix is usually of infinite order, and in principle its eigenvalues and eigenvectors can be used to construct the Green function from the  $\hat{L}$  resolvent matrix. Approximations are usually necessary, at least in the form of truncation of the  $\hat{L}$  matrix, and if one produces a

MCR  
12/8/86

sequence of such matrices of increasing order and calculates the eigenvalues and eigenvectors of these matrices, a sequence of approximations for the  $\hat{L}$  resolvent matrix can be produced. This sequence is mathematically guaranteed to converge to the exact result for the  $\hat{L}$  resolvent matrix (except at its singularities). The accuracy of an approximation depends on the order of the matrix at which the sequence is truncated.

Application of the method to a Hamiltonian representing interactions between fermions and bosons involves complications arising from the large number of terms generated by the commutation properties of boson operators.

This dissertation describes the method and its use in the study of fermion-boson couplings. Approximations to second order in stepping operators are calculated for simplified Froehlich and Lee models. Limited thermodynamic results are obtained from the Lee model. Exact energy eigenvalues are obtained by operator algebra for simplified Froehlich, Lee and Dirac models. These exact solutions comprise the main contribution of this research and will prove to be valuable starting points for further research. Suggestions are made for further research.

## Preface

### Purpose

My original intent in writing this dissertation was primarily to describe the first serious attempt at applying a particular calculational technique, called the Liouville resolvent method, to the study of interactions between fermions and bosons. In particular, I planned to describe how this unconventional method of doing quantum field theory can be used to calculate eigenvalue spectra and even thermodynamic Green functions for simple fermion-boson couplings.

In the course of trying to provide an explanatory background that would be adequate for a thorough understanding of the implementation of the method, I became convinced that it would be worthwhile to put together a comprehensive description, not only of the method and its use, but also of the essential underlying concepts. The many important ideas are scattered through various sources. I endeavored to prepare a write-up that would serve for new students as a satisfactory introduction to the subject, and that would provide conveniently accessible reference material to others, including myself, who want or need to review the subject on occasion. A condensation of this write-up is included in this dissertation as background material.

## Arrangement

The body of the dissertation is divided into chapters, which are subdivided into sections. In accordance with my stated purpose, I have devoted the first nine chapters, comprising about half of the body of the dissertation, to material that is largely derivative from other sources.

Chapter 1 introduces general background for the problem of calculating properties of systems characterized by fermion-boson couplings. Chapter 2 introduces important but simple second-quantized Hamiltonian operators describing systems of interacting fermions and bosons. Chapter 3 surveys existing methods of calculating a Green function, for a second-quantized Hamiltonian operator, and compares the Liouville resolvent method with others. In principle, it is possible to use the Green function to determine the thermodynamics of the system represented by the Hamiltonian.

The next three chapters survey important relevant mathematical concepts. Chapter 4 defines and describes Hilbert spaces. Chapter 5 extends the discussion to operator Hilbert spaces and leads to the Lie algebra of conditional stepping operators. Chapter 6 discusses relevant properties of Lie algebras.

The next triad of chapters explains in detail the Liouville resolvent method. Chapter 7 develops the theory of the method in terms of Green functions. Chapter 8 explains how the method is applied to obtain exact solutions

in simple cases. Chapter 9 explains the techniques of using the method to obtain approximate solutions in more complicated situations.

The three chapters after these demonstrate the use of the method to find Green functions for simple Hamiltonian operators representing systems with fermion-boson couplings. Chapters 10 and 11 show the use of approximation techniques to find the truncations of the Green functions to second order in stepping operators for a simplified Lee and a simplified Froehlich model respectively. Further calculations for the simplified Lee model lead to expectation values of number operators in certain thermodynamic limits. Chapter 12 shows the use of the method to reconstruct a known exact Green function for the simplified Froehlich model, although the Green function is not in an immediately usable form. An attempt to get a usable form seems at first to lead to a new mathematical construct, the operator-valued generalized Bessel function. Chapter 13 summarizes some properties of this function.

A consideration of the displaced harmonic oscillator leads in Chapter 14 to a systematic analysis of the basis states from which the resolvent method builds Green functions. This consideration incidentally shows that the generalized Bessel functions are actually ineffectual.

Chapter 15 introduces projection-operator basis states. Chapters 16, 17 and 18 show how the Liouville

resolvent method, when used with such basis states, gives transition-energy eigenvalues for the simplified Froehlich, Lee and Dirac models, respectively, and leads in particular to the splitting of energy levels characteristic of the Dirac model. After this successful demonstration of the uses of the method in the study of fermion-boson couplings, Chapter 19 suggests some topics for further research, including the construction of Green functions and the calculation of thermodynamic properties for the Hamiltonians of interest.

#### Style

Decimal numbering is used for chapters and sections. A version of the author-date system is used for references.

#### Notation

Condon and Odabasi, on p. 74 of their 1981 book on atomic structure, wrote: "Notation in physics and mathematics is exceedingly important." But, as Goldstein wrote in the preface to the first edition of his text on classical mechanics: "The question of notation is always a vexing one. It is impossible to achieve a completely consistent and unambiguous system of notation that is not at the same time impracticable and cumbersome." Gibbs wrote that his hesitation in regard to the merits of different notations kept him from publishing (Wheeler, L. P. 1962. Josiah Williard Gibbs. New Haven: Yale Univ. Press, paperback ed., chap. 7.)

Notation for summations, integrals, partial and total derivatives, infinite products, and the like, are standardized. Many authors, including Bak, Cropper, Fetter and Walecka, Feynman, Kittel, Landau and Lifschitz, Levich, Liboff, and Park, distinguish quantum-mechanical operators by carat-like circumflexes, and this notation is used here. Three-vectors are denoted here by overhead arrows rather than by bold-face type. It should be possible to infer, from the context, the meanings of any special symbols not explicitly defined.

## Acknowledgements

I began graduate studies with Virginia Tech through the off-campus program at Dahlgren. I thank all of the people who made this program possible, including those members of the faculty who made the long trips to Dahlgren to teach classes.

After obtaining a master's degree, I continued studies off and on campus. During much of the time that I was in residence at the university, I was in a program of full-time advanced study supported by my employer. I thank Dr. David W. Lando for recommending me for this program, and the management and board of directors of the Naval Surface Weapons Center for approving me.

I appreciate the efforts of the members of my dissertation committee, all of whom have taught classes in which I was a student, and all of whom have been helpful in various ways. For many reasons I am particularly grateful to my advisor, Dr. Samuel P. Bowen. He is, I believe, largely responsible for the success of the off-campus degree program in physics. He recruited me into the program, encouraged me to continue graduate studies, and suggested the topic of my dissertation. Through his seemingly tireless dedication and his enthusiasm in the face of adversity, he has been a source of inspiration to me and many others. Most of all, he has been a patient and understanding friend and teacher.



learn physics. For this reason, I dedicate this dissertation to her.

Last but not least, I owe thanks to my four-footed friend, Folly, a very special sheltie. She did not understand why I wanted to leave, but she waited, and remembered, and forgave.

Boson -- a bird-bolt: a blunt or ball-headed arrow.

Boutell's Heraldry

"When I use a word," Humpty Dumpty said, in rather a scornful tone, "it means just what I choose it to mean -- neither more nor less."

"Lewis Carroll", Alice in Wonderland

Of making many books there is no end . . .

Ecclesiastes 12.12

Of making many bosons there is no end!

## Table of Contents

	Page
Abstract . . . . .	ii
Preface. . . . .	iv
Acknowledgements . . . . .	ix
Table of Contents. . . . .	.xiii

### Chapters and Sections

1. Introduction. . . . .	1
1.1. Background . . . . .	1
1.2. Statement of Problem . . . . .	2
1.3. Simplifications. . . . .	3
1.4. Fermion-Boson Couplings. . . . .	4
2. Hamiltonians. . . . .	6
2.1. Froehlich Hamiltonian. . . . .	6
2.2. Dirac Hamiltonian. . . . .	8
2.3. Lee Model. . . . .	9
2.4. General Form . . . . .	10
3. Review of Computational Methods . . . . .	12
3.1. Diagrammatic Expansions. . . . .	12
3.2. Moment Expansions. . . . .	15
3.3. Decoupling Factorizations. . . . .	17
3.4. Functional Derivative. . . . .	19
3.5. Resolvent Equations. . . . .	19
4. Hilbert Spaces. . . . .	21

4.1.	Algebraic Structures . . . . .	21
4.2.	Definition of Hilbert Space. . . . .	21
4.3.	Finite-Dimensional Hilbert Spaces. . . . .	24
4.4.	Infinite-Dimensional Hilbert Spaces. . . . .	25
4.5.	Quantum Dynamics in Hilbert Space. . . . .	27
4.6.	Fock Space . . . . .	29
5.	Operator Hilbert Spaces . . . . .	32
5.1.	Superspaces . . . . .	32
5.2.	Fermi Space. . . . .	33
5.3.	Bose Space . . . . .	34
5.4.	Pontryagin Space . . . . .	36
5.5.	Density Operator . . . . .	38
5.6.	Conditional Operators. . . . .	40
6.	Application of Lie Groups . . . . .	44
6.1.	Algebra. . . . .	44
6.2.	Lie Algebra. . . . .	45
6.3.	Cartan Subalgebra. . . . .	50
6.4.	Group $U(n)$ . . . . .	51
6.5.	Judd Procedure . . . . .	53
7.	Liouville Resolvent Method. . . . .	56
7.1.	Green Functions. . . . .	56
7.2.	Liouville Operator . . . . .	62
7.3.	Moment Expansion of Green Function . . . . .	65
7.4.	Resolvent. . . . .	67
7.5.	Moment Expansion of Resolvent. . . . .	69

8.	Application of the Liouville Resolvent Method . . .	72
8.1.	Evaluation of Diagonal Hamiltonians. . . . .	72
8.2.	Spectral Function. . . . .	77
9.	Approximate Solutions . . . . .	83
9.1.	Discussion . . . . .	83
9.2.	Truncation Approximations. . . . .	85
9.3.	Feenberg Formulas. . . . .	87
9.4.	Summary of Method. . . . .	89
9.5.	Solutions to First Order . . . . .	91
9.6.	Partial Solution to Second Order . . . . .	94
9.7.	Relation of Zubarev and Liouville Methods. . .	95
10.	Truncated Solution for Lee Model. . . . .	97
10.1.	Specification of Basis States. . . . .	97
10.2.	Calculation of Inner Products. . . . .	98
10.3.	Calculation of Resolvent Matrix Elements.. . .	99
10.4.	Construction of Green Functions. . . . .	100
10.5.	Calculation of Particle Number . . . . .	101
10.6.	Evaluation of the Binding Energy Term. . . . .	103
10.7.	Evaluations for Thermodynamic Limits . . . . .	106
11.	Truncated Solution for Froehlich Model. . . . .	108
11.1.	Specification of Basis States. . . . .	108
11.2.	Proof Relating to Coupling Factor. . . . .	109
11.3.	Application of Liouville Superoperator . . . .	110
11.4.	Calculation of Inner Products. . . . .	111
11.5.	Calculation of Resolvent Matrix Elements . . .	112

11.6.	Calculation of Matrix Elements . . . . .	112
11.7.	Calculation of Green Function. . . . .	115
11.8.	Use of Summed Basis States . . . . .	116
11.9.	Summed Basis States in Pontryagin Space. . . . .	118
12.	Mahan's Independent Boson Model . . . . .	121
12.1.	Operator Similarity Transformations. . . . .	121
12.2.	Canonical Transformation of Hamiltonian. . . . .	122
12.3.	Green Function . . . . .	124
12.4.	Boson Factors. . . . .	126
12.5.	Displacement Operator. . . . .	127
12.6.	Campbell-Baker-Hausdorff Theorem . . . . .	127
12.7.	Expansion of Boson Factor. . . . .	128
12.8.	Rearrangement of Double Sum. . . . .	128
13.	Generalized Bessel Functions. . . . .	131
13.1.	Definition . . . . .	131
13.2.	Generating Function. . . . .	131
13.3.	Simple Properties. . . . .	132
13.4.	Recursion Relations. . . . .	133
13.5.	Commutation Relations. . . . .	134
13.6.	Miscellaneous Properties . . . . .	136
14.	Simple Boson Factors. . . . .	138
14.1.	Displaced Harmonic Oscillator. . . . .	138
14.2.	Use of Displacement Operator . . . . .	138
14.3.	Boson Subfactors . . . . .	141
14.4.	Use of Generalized Bessel Functions. . . . .	145

15.	Projection-Operator Boson Factors . . . . .	147
15.1.	Projection-Operator Basis States . . . . .	147
15.2.	Evaluation of Expectation Value. . . . .	149
15.3.	Associated Laguerre Polynomials. . . . .	151
16.	Einstein and Simplified Dirac Models. . . . .	153
16.1.	Simple Solution of Einstein Model. . . . .	153
16.2.	Projection-Operator Solution . . . . .	155
16.3.	Solution of Simplified Dirac Model . . . . .	158
17.	Lee Model . . . . .	163
17.1.	Factorization of Basis State . . . . .	163
17.2.	Fermion Factor . . . . .	163
17.3.	Boson Factor . . . . .	165
17.4.	Matrix Solutions . . . . .	167
17.5.	Eigenvalue Problem . . . . .	168
17.6.	Eigenvalues for Lee Model. . . . .	170
18.	Dirac Model . . . . .	172
18.1.	Basis State. . . . .	172
18.2.	Calculation of Boson Factors . . . . .	172
18.3.	Fermion Factors. . . . .	174
18.4.	Matrix Equation. . . . .	175
18.5.	Matrix Equation for Alternate Basis State. . .	177
18.6.	Eigenvalues. . . . .	178
19.	Suggested Topics for Continued Effort . . . . .	181
19.1.	Other Fermion Basis States . . . . .	181
19.2.	Green Functions for Summed Basis States. . . .	182

19.3. Differential Operators . . . . .	186
19.4. Thermodynamics of Realistic Systems. . . . .	186
Literature Cited . . . . .	190
Vita . . . . .	198

## 1. Introduction

### 1.1. Background

One of the basic problems in physics is determining the thermodynamics of systems composed of particles interacting with fields. All of the important thermodynamic properties of a quantum-mechanical system described by a Hamiltonian operator can be found from the thermodynamic potential. The thermodynamic potential can be found if an appropriate Green function can be specified for the system. The Green function is much used in classical mechanics as an expression that characterizes the linear response of the system. It is the solution to a differential equation modeling such a response, and its form depends on the boundary conditions. In quantum field theory, non-linear Green functions are used (Abrikosov et al. 1963).

Green functions can be calculated exactly only for very simple Hamiltonian operators, and usually eigensolutions can be found for such operators without the need for Green functions. For most systems of interest, the Green functions must be calculated by some method of approximation. A well-known example of such methods involves diagrammatic expansions, but a few other methods exist. All have limitations (Bowen 1975). One troublesome weakness common to all but one of these schemes is the lack of any systematic technique for improving the approximation

so as to ensure convergence of the solution towards the exact physical result.

A convergent method of calculating approximate thermodynamic Green functions for a given Hamiltonian has been developed in principle (Bowen 1975). The method, to be referred to as the Liouville resolvent method, involves the construction of a sequence of approximants that converges for coupling constants of any magnitude. For some very simple Hamiltonians, exact solutions can be obtained (Bowen et al. 1984).

The method has been used successfully to obtain approximate solutions for some simple Hamiltonians, particularly the Anderson model (Bowen 1978) and, more recently, the Hubbard model.

Attempts to apply the method to systems involving bosons encounter difficulties, arising mathematically from a proliferation of terms generated by the commutation properties of boson operators, and related physically to the proliferation of bosons permitted in interactive processes by the inapplicability of the Pauli exclusion principle to bosons.

## 1.2. Statement of Problem

The subject of this dissertation is an investigation of part of the eigenvalue spectra of some simple Hamiltonians that have coupling between the degrees of freedom for

fermions and bosons. The excitation spectra and thermodynamics of these Hamiltonians are explored by means of the Liouville resolvent method and operator algebras. In this approach, the excitations are described by second-quantized stepping operators that are eigenvectors of the quantum-mechanical Liouville operator. This operator is closely related to the thermodynamic Green function, from which it is possible to calculate the thermodynamics of coupled many-particle systems. The object of the research undertaken for this dissertation was to study the connection between the quantum-mechanical Liouville operator and the thermodynamic Green functions for some simple Hamiltonians describing coupled many-particle systems, to find the eigenvectors of the operator, and to determine the equations from which the thermodynamics of the systems can be found.

### 1.3. Simplifications

The simplest Hamiltonians that have coupling between fermions and bosons are those that contain linear powers of boson stepping operators, and only such Hamiltonians are considered here.

Because the goal of the described research was not simply to manipulate the algebra of operators, but to illuminate the physics of coupled many-particle systems, the Hamiltonians of interest were for most purposes restricted to fermion-boson couplings with a single boson mode, with no

summation over different momentum states for the bosons. This restriction simplified calculations while retaining the essential physics.

#### 1.4. Fermion-Boson Couplings

Elementary particles can be divided into two types on the basis of the statistical properties of their interactions with other particles of the same type. These statistical properties are associated with the Pauli exclusion principle. Fermions are subject to this principle, bosons are not. The interaction between a charged particle and a radiation field can be said to be an interaction between a fermion and bosons. Interactions between constituent particles of a material medium are often thought of as being mediated by other particles, in which case the constituent particles are often fermions and the mediating particles are bosons.

The most common example in condensed-matter physics of the interaction between fermions and bosons is the interaction in a crystal between an electron and a vibration of the crystal lattice. The state of the electron is described by a wave function. The vibration is described by an eigenstate of the phonon. The vibration is a disturbance of the lattice by the phonon in which atoms in the crystal are perturbed from their equilibrium positions. The perturbation distorts the lattice, changing the effective

electrostatic potential in the crystal, thereby possibly deflecting and scattering the electron (Ziman 1960:175; Harrison 1970).

"Second" quantization essentially transfers quantization from states to operators. The description of systems in "second"-quantized form (March et al. 1967; Baym [1969] 1974) and the use of stepping operators in Fock space is ubiquitous in many-particle theory. The stepping operators for quantized vibrational modes in solids are essentially like the ladder operators for a simple harmonic oscillator. The number of particles in an oscillator state corresponds to the degree of excitation of the oscillator. In non-relativistic many-particle theory, particles cannot be created or destroyed (Kaempffer 1965), but if the grand canonical ensemble is used, the number of particles can change as particles enter or leave the system.

## 2. Hamiltonians

### 2.1. Froehlich Hamiltonian

The Froehlich Hamiltonian operator is used to describe the interaction between an electron and phonons in a solid, and is particularly used to model what is called the Froehlich polaron. The derivation of the expression for the operator requires several assumptions. Essentials of the derivation are given in various sources (Fetter and Walecka 1971; Haken 1973, 1976; Haken 1976; Mahan 1981). In second-quantized form, with summation over spin and wave-vector states, the operator is written (using notation that is commonly though not universally employed) as

$$\hat{H} = \sum_{\vec{k}, \sigma} \hbar \epsilon_{\vec{k}} \hat{c}_{\vec{k}, \sigma}^{\dagger} \hat{c}_{\vec{k}, \sigma} + \sum_{\vec{q}} \hbar \omega_{\vec{q}} \hat{a}_{\vec{q}}^{\dagger} \hat{a}_{\vec{q}}$$

$$+ \sum_{\vec{k}, \vec{q}, \sigma} \hbar \omega_{\vec{q}} \lambda_{\vec{q}} \hat{c}_{\vec{q}, \sigma}^{\dagger} \hat{c}_{\vec{k}+\vec{q}, \sigma} (\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^{\dagger}).$$

Some aspects of this expression may be clarified by the following relationships:

$$E_c = \hbar \epsilon_{\vec{k}} = \frac{\hbar^2 k^2}{2m} = \frac{p^2}{2m} = \frac{(-i\hbar \vec{\nabla}) \cdot (-i\hbar \vec{\nabla})}{2m} = -\frac{\hbar^2 \nabla^2}{2m}$$

for free electrons,

$$E_a = \hbar \omega_{\vec{q}}$$

$$E_I = \hbar \omega_{\vec{q}} \lambda_{\vec{q}} = M_{\vec{q}}$$

The coupling coefficient  $\lambda$  is here assumed to have a

possible dependence on the momentum states of the phonons. The Froehlich Hamiltonian operator is related to the Fourier transform of the first derivative, with respect to the nuclear displacements, of the one-electron interaction between the ions and the conduction electrons.

If it is assumed that interaction with the phonon or hole does not change the state of the electron, then the system can be modeled by a simpler version of the Froehlich Hamiltonian operator, written as

$$\hat{H} = \hbar\epsilon_c \hat{c}^\dagger \hat{c} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} + \sum_{\vec{q}} \hbar\omega_{\vec{q}} \lambda_{\vec{q}} \hat{c}^\dagger \hat{c} (\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^\dagger).$$

Physicists (Mahan 1981) have found exact solutions for this in a number of ways. For a constant coupling coefficient, the expression reduces to a particularly simple form.

The simplest useful variant of the Froehlich Hamiltonian operator, for a single phonon frequency, is sometimes called the Einstein or independent boson model (Mahan 1981). This simplified form of the Froehlich Hamiltonian operator was used in the research to be discussed. It is written

$$\hat{H} = \hbar\epsilon_c \hat{c}^\dagger \hat{c} + \hbar\omega_0 \hat{a}^\dagger \hat{a} + \hbar\omega_0 \lambda_0 \hat{c}^\dagger \hat{c} (\hat{a} + \hat{a}^\dagger).$$

Theoretical physicists working in relativistic quantum

field theory and in the theory of elementary particles often choose for convenience a system of units in which universal constants such as the speed of light in a vacuum and Planck's quantum of action are dimensionless and of unit magnitude (Jackson 1975). Planck's quantum of action is often chosen to be unity in many-body theory, also. When Dirac's reduced Planck's constant  $\hbar$  is unitized, the Einstein model reduces to

$$\hat{H} = \epsilon_c \hat{c}^\dagger \hat{c} + \omega_0 \hat{a}^\dagger \hat{a} + \omega_0 \lambda_0 \hat{c}^\dagger \hat{c} (\hat{a} + \hat{a}^\dagger).$$

## 2.2. Dirac Hamiltonian

A simple Hamiltonian operator representing a two-level electronic system, with two different electronic states created by two distinct fermion stepping operators, interacting with boson modes, is

$$\begin{aligned} \hat{H} = & \hbar \epsilon_c \hat{c}^\dagger \hat{c} + \hbar \epsilon_b \hat{b}^\dagger \hat{b} + \sum_{\vec{q}} \hbar \omega_{\vec{q}} \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} \\ & + \sum_{\vec{q}} \hbar \omega_{\vec{q}} \lambda_{\vec{q}} (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) (\hat{a}_{\vec{q}} + \hat{a}_{-\vec{q}}^\dagger). \end{aligned}$$

Operators essentially like this have been used to study the two-level molecular polaron (Rivier and Coe 1977; Hewson 1981; Stolze and Brandt 1983). This is also the Dirac Hamiltonian operator, if an alternate interpretation is made of the two distinct fermion stepping operators; namely, that one of them creates electrons while the other creates holes.

A simplified Dirac Hamiltonian operator, with no summation over radiation modes, was used in the research to be discussed. With Dirac's reduced Planck's constant of unity, it is written as

$$\hat{H} = \epsilon_c \hat{c}^\dagger \hat{c} + \epsilon_b \hat{b}^\dagger \hat{b} + \omega_0 \hat{a}^\dagger \hat{a} \\ + \omega_0 \lambda_0 (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) (\hat{a} + \hat{a}^\dagger).$$

### 2.3. Lee Model

A simpler version of the original Dirac Hamiltonian operator is the Lee model, which is written as

$$\hat{H} = \hbar \epsilon_c \hat{c}^\dagger \hat{c} + \hbar \epsilon_b \hat{b}^\dagger \hat{b} + \sum_{\vec{q}} \hbar \omega_{\vec{q}} \hat{a}_{\vec{q}}^\dagger \hat{a}_{\vec{q}} \\ + \sum_{\vec{q}} \hbar \omega_{\vec{q}} \lambda_{\vec{q}} (\hat{c}^\dagger \hat{b} \hat{a}_{\vec{q}} + \hat{b}^\dagger \hat{c} \hat{a}_{\vec{q}}^\dagger).$$

Although this has two distinct fermion stepping operators, it differs from the original Dirac Hamiltonian operator by having restrictions on the fermion couplings. As the Jahn-Teller model, this operator is another one of those that have been used to describe the interaction of two-level atoms with phonons (Crowne 1983). As the Wigner-Weisskopf model, the operator has been used to model a two-level atom in a massless boson radiation field (Davidson and Kozak 1970a, 1970b). Physicists have found state and scattering matrices for the Lee model in several ways. Exact results have been obtained for certain restricted conditions

(Schweber 1961).

A simplified Lee model with no summation over boson states was used in the research to be discussed. With a Dirac's reduced Planck's constant of unity, it is written

$$\hat{H} = \epsilon_c \hat{c}^+ \hat{c} + \epsilon_b \hat{b}^+ \hat{b} + \omega_0 \hat{a}^+ \hat{a} \\ + \omega_0 \lambda_0 (\hat{c}^+ \hat{b} \hat{a} + \hat{b}^+ \hat{c} \hat{a}^+).$$

#### 2.4. General Form

All of the simplified Hamiltonian operators mentioned may be thought of as particular cases of the Hamiltonian operator

$$\hat{H} = \epsilon_b \hat{b}^+ \hat{b} + \epsilon_c \hat{c}^+ \hat{c} + \hbar \omega_0 \hat{a}^+ \hat{a} \\ + \lambda_{ob} \hbar \omega_0 \hat{c}^+ \hat{b} \hat{a}^+ + \lambda_{ob} \hbar \omega_0 \hat{b}^+ \hat{c} \hat{a} \\ + \lambda_{oc} \hbar \omega_0 \hat{c}^+ \hat{b} \hat{a} + \lambda_{oc} \hbar \omega_0 \hat{b}^+ \hat{c} \hat{a}^+.$$

The Dirac model is the most general of these cases, with a single value of the fermion-boson coupling coefficient. In the Lee model, one form of the coupling coefficient vanishes. In the Einstein model, only a single type of fermion occurs. The loss of a pair of terms involving fermion-boson couplings in the Lee model means that this model lacks a symmetry that is shared by the Dirac and Einstein models. The general form of the Hamiltonian operator allows the different symmetry characteristics of

the particular cases to be seen at a glimpse, but because of these characteristics, it is not a useful starting point for calculations.

### 3. Review of Computational Methods

#### 3.1. Diagrammatic Expansions

A review of those methods that are used in quantum field theory to do approximate calculations of Green functions may as well begin with the method of diagrammatic expansions. This method, in one form or another, has had a pervasive influence on all branches of modern physics. Explanations of the derivation and use of the method can be found at varying levels of detail and in various contexts. In addition to works concentrating on nonrelativistic many-particle theory (e.g. Abrikosov et al. 1963; Fetter and Walecka 1971; Rickayzen 1980; Mahan 1981; cf. Kirzhnits 1967; March et al. 1967; Inkson 1967), suitable references include books oriented towards relativistic quantum field theory (e.g. Mandl 1959; Bjorken and Drell 1964, 1965; Sakurai 1967; Ziman 1969; Mandl and Shaw 1985), especially those introducing many-body techniques before adding the complexities of special relativity (e.g. Schweber 1961; Roman 1965). Recent works, though less apt than earlier ones to be outdated with respect to some details, tend to have formal and specialized treatments of the method. The books that best cover the method necessarily emphasize techniques over applications, because the material that must be presented is lengthy (Anderson 1984:2-3).

Typically, the method is applied to a double-time

single-particle Green function expressed in terms of time-ordered stepping operators. When the operators are put into the interaction representation, factors of the time-development operator are introduced. These factors involve exponentials of the noninteracting part of the Hamiltonian operator. The time-development operator is then expanded in perturbation series, which lead to scattering matrices appearing in numerator and denominator of the expression for the Green function.

Wick's theorem is used to sort the time-ordered operators into products of paired terms. The resulting terms are depicted by diagrams, such as the Feynman diagrams. The terms are sorted into classes based on topological similarities of the diagrams. The sorting is facilitated by the use of the diagrams, because the salient similarities can be perceived more easily among the diagrams than among the corresponding terms in a complicated expression.

The class of disconnected diagrams, representing vacuum polarization terms, is used to eliminate the denominator of the expression for the Green function by cancelling the terms of the scattering matrix in the denominator. Partial summation of the remaining classes of diagrams is then used to characterize and approximate the entire series expansion in the expression representing the Green function.

The resulting expression for the Green function can be used to obtain Dyson's equation by making a Fourier transform of the Green function from time dependence to energy dependence. For thermodynamics at finite temperatures, time and temperature are considered parts of a complex variable. An analytic continuation of frequencies from the imaginary to the real axis then generates the retarded Green function known as the Matsubara Green function.

For purposes of calculation, a system with interactions is often modeled simply by a perturbed Hamiltonian, which is constructed by adding, to the ground state Hamiltonian operator, a perturbation describing the interaction. As has been mentioned, the Green function for the system is expanded in terms of the perturbation part of the Hamiltonian operator. As a result, it is possible for the expansion to be asymptotic or not convergent. Convergence may not occur at all for interactions with large coupling coefficients (Dirac 1978:20, 1978:36-37; Schwarzschild 1985).

If the coupling coefficient is small, as it is for the electromagnetic interaction, the terms in the expansion for the Green function can be arranged, with the aid of diagrams, in powers of the coupling coefficient. An infinite number of higher-order terms are then considered to

be negligible. Because a finite or summably infinite number of terms remains, it becomes possible to do actual computations.

This practice in effect depends on the assumption that some classes of diagrams are less important than others, and that these less important ones, and the terms they represent, can be summarily ignored. This assumption can be open to question (ter Haar 1985). "Contrary to what one is sometimes led to believe, the Feynman-diagram techniques do not prove that the large individual contributions we evaluate are not swamped by the sum of the overwhelmingly larger number of diagrams we dismiss."

Most of natural science, including biology, chemistry, and much of condensed-matter and atomic physics, involves primarily phenomena arising from the electromagnetic interaction, but these phenomena can be highly correlated, so that the validity of expansions in terms of the ground-state properties of the noninteracting part of the Hamiltonian operator becomes suspect (Kadanoff and Martin 1961). Any attempt to simplify the expansion by including part of the correlation in the unperturbed Hamiltonian invalidates Wick's theorem and necessitates a mean-field approximation (Abraham and Robert 1980).

### 3.2. Moment Expansions

The method of moment expansions is grounded in the

classical theory of mathematical moments (Lonke 1971). This method, as well as the method of decoupling factorizations and the Liouville resolvent method, would typically be applied to a single-particle retarded Green function. The spectral function associated with the Green function is expanded as a sum of moments of successive orders. This moment expansion is approximated by some variant of Pade approximants, which are essentially ratios of polynomials (Lonke 1971; Masson 1970). The approximation is analytically continued for small denominators in the expansion.

Although the individual moments are rigorously exact, the expansion representing the spectral weight function consists of an infinite number of moments. Finite Pade approximants yield a finite number of terms, so that there are finitely many poles in the polynomial solution, and countably many moments in the expansion. Any practical calculation must be done using only part of the total spectrum of moments.

The thermodynamic limit is of considerable importance in quantum field theory. In the thermodynamic limit, extensive quantities become infinite while intensive quantities remain finite, and the spectral function becomes continuous. From finitely many moments, however, it is not possible to generate a continuous spectrum in the

thermodynamic limit.

In spite of its limitations, the method of moment expansions is relevant to subsequent discussions because the technique of moment expansions is used in the development of the Liouville resolvent method.

### 3.3. Decoupling Factorizations

The method of decoupling factorizations is applicable as a mathematical model for mean-field theories in condensed-matter physics (Zubarev 1960). The method has been used successfully to describe magnetism, superconductivity, phase transitions, and various thermal phenomena in systems with components that are highly correlated through interactions.

In this method, a single-particle retarded Green function is explicitly expressed in terms of equilibrium ground-state averages of operators. The Fourier transform of the equation of motion for the Green function is used to generate an infinite hierarchy of equations involving correlation functions. Some higher-order correlation functions are approximated by products of equal-time averages of operators and lower-order correlation functions. By this process, the hierarchy of equations is approximated by a closed non-linear set, and a self-consistent solution is sought for the expectation values (Bowen 1975).

The method of decoupling factors has been subjected to

criticism (Adomian 1971). The factorization process fails to give satisfactory approximations for those large fluctuations of higher-order correlation functions that can occur when mean-field theory fails. In any case, there exists no satisfactory way of systematically employing physical considerations to decide on appropriate factorizations and important approximations. One reference, in discussing equations of motion of the Fourier transform of the Green function, provides a simple example of the difficulty (Haken 1976:278). "The example shows clearly how easy it is to make mistakes in the use of Green's functions, and that we need a considerable 'feel' for the physics of the situation when using them. There are in fact cases in the literature where the wrong approximations have been made, particularly with regard to the way factorization has been carried out."

As will be demonstrated in a later chapter, what is of interest regarding this method is that, if there were some systematic way of finding appropriate decoupling factorizations, the method would become effectively equivalent to the Liouville resolvent method.

### 3.4. Functional Derivative

The method of the functional derivative is like the method of diagrammatic expansions in that it is applied to a double-time single-particle Green function expressed in terms of time-ordered stepping operators in the interaction representation. The method of the functional derivative is like the method of decoupling factorizations in that the Green function is assumed to obey an equation of motion. The equation of motion is made a function of some arbitrary scalar potential that serves as an artificial variational parameter. Then the Green function itself has some dependence on this parameter. The equation of motion is thus a single differential equation for the Green function, and can be solved iteratively (Kadanoff and Baym 1962). The Green function conveniently obeys the same differential equation and boundary conditions as an equilibrium Green function. Unfortunately, no systematic treatment of regions of convergence in perturbative solutions seems to be available.

### 3.5. Resolvent Equations

The method of resolvent equations, to be referred to as the Liouville resolvent method, is based on finding approximants for the Fourier transform of a single-particle retarded Green function. The method is characterized, not, for example, by diagrams selected and summed to some finite

or infinite order in the coupling coefficient for an interaction, but instead by primitive basis states that are conditional generalized stepping operators representing physical transitions between states of motion. The implementation of the method involves the construction of a sequence of approximants consisting of a series of larger and larger matrices, with each matrix in succession involving more conditional operators. A solution is found by matrix-algebraic techniques.

The most significant attribute of the method of resolvent equations sets this method apart from all of the others that have been reviewed in the preceding sections. A mathematical theorem derived by the techniques of functional analysis guarantees that the sequence of approximants to the exact resolvent matrix element converges for any magnitude of the coupling coefficient in the Hamiltonian (Masson 1970). However, the convergence could be slow unless the relevant energy scale is large enough to render details of the spectral function unimportant. A figure of merit for any finite truncation of the sequence of approximants is an experimentally determined resolution parameter in the spectral function (Bowen 1975). If fine detail of the spectral function is smaller in scale than the resolution parameter and hence is not resolvable, the coarser structure can be well represented by a finite matrix.

## 4. Hilbert Spaces

### 4.1. Algebraic Structures

In order to understand the Liouville resolvent method, it is necessary to have some familiarity with the properties of the manifolds used in the discussion of the theory underlying the method. Although treatments of abstract mathematical spaces can be found in texts on modern analysis, a brief summary of some relevant terminology may serve as a helpful introduction to the subject, especially because some of the spaces that are of interest are not mentioned in elementary texts and are discussed only in the specialized literature.

A linear vector space is an additive Abelian group (Simmons 1963) distinguished by an additional operation called scalar multiplication. In a linear vector space, the elements can be multiplied by numbers, according to the operation of scalar multiplication, but not necessarily by one another. The elements of a linear vector space are called vectors. Any set of linearly independent vectors in the space can form a basis for the space. Other vectors in the space can be constructed from linear combinations of scalar multiples of the basis vectors.

### 4.2. Definition of Hilbert Space

Let  $\|x\|$  be the distance from the element  $x$  to the origin of a linear vector space  $L$ . Such a distance is

called a norm, and has the following properties:

- (1)  $\|x\| \geq 0$ ,
- (2)  $\|x\| = 0 \Leftrightarrow x = 0$ ,
- (3)  $\|x + y\| \leq \|x\| + \|y\|$ ,
- (4)  $\|\alpha x\| = |\alpha| \|x\|$ ,  $\alpha$  a scalar.

A normed linear vector space is a linear vector space on which a norm is defined.

A metric  $d(x, y)$  on  $L$  satisfies the following conditions:

- (1)  $d(x, y) \geq 0$ ,
- (2)  $d(x, y) = 0 \Leftrightarrow x = y$ ,
- (3)  $d(x, y) = d(y, x)$ ,
- (4)  $d(x, y) \leq d(x, z) + d(z, y)$ .

A metric converts  $L$  into a metric space. Different metrics convert  $L$  into different metric spaces. The properties of the norm give rise to a particular induced metric. A normed linear vector space is a metric space with respect to this induced metric, which is

$$d(x, y) = \|x - y\|.$$

Let  $\{x_n\}$  be a sequence of points in a metric space  $X$ . The sequence converges with a point in the space as a limit, if the set of points in the sequence has a limit point in the set; that is, if

$$\exists x \in X \exists \forall \epsilon > 0 \exists n_0 > 0 \exists n \geq n_0$$

$$\Rightarrow d(x_n, x) < \varepsilon.$$

A Cauchy sequence is intrinsically convergent; that is,

$$\forall \varepsilon > 0 \exists n_0 > 0 \exists m, n \geq n_0 \Rightarrow d(x_n, x_m) < \varepsilon.$$

A space that is complete as a metric space is one in which every Cauchy sequence is convergent to a vector in the space.

A Banach space is a normed linear vector space that is complete as a vector space.

An inner product, of the form  $(x, y)$ , of two vectors has the following properties:

$$(1) \quad (\alpha x + \beta y, z) = \alpha \cdot (x, z) + \beta \cdot (y, z),$$

$$(2) \quad (x, y)^* = (y, x),$$

$$(3) \quad (x, x) = \|x\|^2.$$

A Hilbert space is a special type of complex Banach space that has a norm arising from an inner product. Associated with the inner product is the concept of an angle between two vectors. This feature of a Hilbert space is of importance because it provides a way of determining whether or not vectors are orthogonal.

The existence and properties of the inner product permit a classification of operators on a space. Operators produce transformations of normed linear vector spaces.

Consider an example. Any Hilbert space has many possible bases. Unless otherwise indicated, a basis for a

Hilbert space is usually chosen to be some set of orthonormal vectors or functions. The orthonormality can be established by the inner product. A unitary operator transforms from one orthonormal basis to another. It changes the components of any state vector, but in a way that preserves inner products by maintaining the length of a vector and the angle between two vectors.

#### 4.3. Finite-Dimensional Hilbert Spaces

Cartesian space is a special example of a type of linear vector space denoted by  $l_p^n$ . An element of  $l_p^n$  is a vector

$$\mathbf{x} = (x_1, x_2, \dots, x_n)$$

that is an n-tuple of scalars. The inner product of two vectors

$$\mathbf{x} = (x_1, x_2, \dots, x_n),$$

$$\mathbf{y} = (y_1, y_2, \dots, y_n),$$

in  $l_p^n$  is defined by

$$(\mathbf{x}, \mathbf{y}) = \sum_{i=1}^n x_i^* y_i$$

and gives rise to a norm calculated by

$$\|\mathbf{x}\| = \left[ \sum_{i=1}^n |x_i|^p \right]^{1/p}.$$

In general,  $(\mathbf{x}, \mathbf{y})$  is a complex number, and the inner

product cannot be expressed in terms of an angle between  $x$  and  $y$ , but the concept of orthogonality holds. The condition for orthogonality of  $x$  and  $y$  is

$$(x, y) = 0.$$

#### 4.4. Infinite-Dimensional Hilbert Spaces

The complex abstract Hilbert spaces used in quantum mechanics are usually infinite-dimensional. In a matrix representation of quantum mechanics, operators are represented by infinite square matrices, and vectors are represented by infinite row or column matrices. In the Dirac notation, a row vector  $\phi$  is written as the bra symbol  $\langle\phi|$ , a column vector  $\psi$  is written as the ket symbol  $|\psi\rangle$ , and the inner product of the two is written as  $\langle\phi|\psi\rangle$ . Consider the linear functional for the vector  $\langle\psi|$ , written as

$$F_{\psi}(p) = (\psi, \phi).$$

The value of this linear functional for the vector  $|\phi\rangle$  is also written as  $\langle\phi|\psi\rangle$ . The kets are in Hilbert space; the bras are in another, a dual space. Hilbert space is self-dual, however; it is equivalent to its dual. The adjoint of an operator is in the dual space (Hutson and Pym 1980).

In quantum-mechanics, the elements of the space, although they are called vectors, are usually functions, and the Hilbert space is a function space of the kind sometimes denoted by  $L_p$ .

The important distinguishing characteristics of the typical quantum-mechanical Hilbert space  $H$ , the elements of which are functions (denoted by  $\phi$  or  $\psi$ , for example), can be summarized by four statements (Liboff 1980).

First,  $H$  is linear:

$$(a \text{ is constant}) \vee (\phi \in H) \vee a\phi \in H;$$

$$\phi, \psi \in H \Rightarrow \phi + \psi \in H.$$

Second, there is an inner product:

$$\exists \langle \phi | \psi \rangle \vee \phi, \psi \in H.$$

For the example of functions defined in the one-dimensional interval  $a \leq x \leq b$ , the inner product is

$$\langle \phi | \psi \rangle = \int_a^b \phi^* \psi \, dx.$$

Third, an element has a norm (length)  $\|\phi\|$ , found from the inner product by the relation

$$\|\phi\|^2 = \langle \phi | \phi \rangle.$$

Fourth,  $H$  is complete (Messiah 1968:165-166). Every Cauchy sequence of functions in  $H$  converges to an element of  $H$ . A Cauchy sequence of functions  $\phi \in H$  is such that

$$\lim_{n, m \rightarrow \infty} \|\phi_n - \phi_m\| = 0.$$

The completeness of  $H$  loosely means that  $H$  contains all of its limit points.

In a finite-dimensional space, an orthonormal set is automatically complete. In an infinite-dimensional space,

the completeness requirement must be added to the orthogonality condition (Merzbacher 1970:324).

The infinite-dimensional Hilbert spaces used in elementary quantum mechanics are usually taken to be separable (Messiah 1968:1.248; Jordan 1969; cf. Dirac 1958:40, 1966:1-8; Jammer 1966:321). A Hilbert space is separable if it has an orthonormal basis that consists of a finite or countably infinite number of vectors (Jordan 1969). Then, any orthonormal basis is countable (Riesz and Nagy 1955:197), so that, by definition, norms and inner products have finite values. More generally, a separable space is a topological space that has a countable dense subset (Simmons 1963); that is, it contains a countable dense set of vectors. A vector space is separable (Powell and Crasemann 1965) if any square-integrable function (Byron and Fuller 1969:1.124) is a limit, in the mean, of a converging Cauchy series of square-integrable functions (Messiah 1968:1.160). In particular, a space  $L_2$  of square-integrable functions is a separable Hilbert space (Riesz and Nagy 1955:197).

#### 4.5. Quantum Dynamics in Hilbert Space

Hilbert space provides the mathematical setting for quantum mechanics. Measurable physical observables are represented in the space by operators called dynamical variables, and physical states are functions called state

vectors.

In the Heisenberg picture of quantum mechanics, the time dependence of an operator  $\hat{\mu}_H$  is given by (Haken 1976:125):

$$\hat{\mu}_H(t) = e^{i\hat{H}t/\hbar} \hat{\mu}_H(0) e^{-i\hat{H}t/\hbar}.$$

Differentiation of this expression with respect to time shows that the equation of motion for the operator in the Heisenberg picture is

$$\frac{d\hat{\mu}_H(t)}{dt} = \frac{i}{\hbar} [\hat{H}, \hat{\mu}_H(t)].$$

In the Heisenberg picture, then, the dynamical variables  $\hat{\mu}_H$  vary with time according to Heisenberg's equations of motion (Merzbacher 1970),

$$i\hbar \frac{d\hat{\mu}_H}{dt} = [\hat{\mu}_H, \hat{H}].$$

In the Schroedinger picture, it is the state vectors  $|A_S\rangle$  that vary with time according to the equations

$$i\hbar \frac{d}{dt} |A_S\rangle = \hat{H} |A_S\rangle.$$

The fixed dynamical variables in the Schroedinger picture are related to the time-dependent dynamical variables in the Heisenberg picture by the equation

$$\hat{\mu}_S = e^{-i\hat{H}t/\hbar} \hat{\mu}_H e^{i\hat{H}t/\hbar} .$$

The fixed state vectors in the Heisenberg picture are related to the time-dependent state vectors in the Schroedinger picture by the equation

$$|A_S\rangle = e^{-i\hat{H}t/\hbar} |A_H\rangle .$$

#### 4.6. Fock Space

A single particle in a single spatial dimension can require an uncountably infinite number of dimensions in a system space such as Hilbert space. A state at  $x'$  differs from a state at  $x''$ . Distinct states are in one-to-one correspondence with the continuum of real values of  $x$ .

A system containing  $n$  particles in physical space has a system space with a dimensionality equal to that of the one-dimensional continuum raised to the power  $3n$ .

Consider a hierarchy of sets of basis vectors for infinite-dimensional vector spaces, arranged in order of increasing complication of the sets:

(1)  $n$  countably infinite linearly independent basis vectors;

(2) linearly independent basis vectors labelled by  $m$  indices, each with an infinite range of discrete values  $n$ , spanning a space of  $n^m$  dimensions;

(3) linearly independent basis vectors labelled by  $m$

finite indices, each with a continuous range of values;

(4) linearly independent basis vectors labelled by an infinite number of continuous variables, spanning a space of  $n^m$  dimensions, where both  $m$  and  $n$  are uncountably infinite.

The basis vectors of the usual Hilbert space of the kind  $L_2(\vec{R}^{3n})$  are square-integrable functions over a configuration of  $n$  particles.

The Fock space (March et al. 1967) used in quantum field theory describes an infinite number of states, with each state  $i$  having an indefinite occupation number  $n_i$  of particles in the state (Condon and Odabasi 1981).

Assume that a complete set of dynamical variables  $\hat{U}$  for a single particle can be used also for a system of  $n$  identical particles, even if there are interactions among the particles. Then every eigenvalue  $\mu_i$  of  $\hat{U}$  corresponds to an occupation number operator  $\hat{N}_i$ . The eigenvectors of  $\hat{N}_i$  itself are occupation numbers  $n_i$ .

Assume further that the  $\hat{N}_i$  form a complete set of commuting Hermitian operators for a system of identical particles.

Let kets of the form  $|n_1, n_2, \dots\rangle$  comprise a complete set of orthonormal basis vectors spanning a linear vector space for a system of identical particles. General state vectors for the system can be constructed from linear combinations of multiples of the basis vectors.

The basis vectors respectively assign the eigenvalue  $\mu_1$  to a number  $n_1$  of particles, the eigenvalue  $\mu_2$  to a number  $n_2$  of particles, and so on.

The vacuum state can be written as

$$\Psi^{(0)} = |0, 0, \dots\rangle.$$

One-particle states can be written as

$$\begin{aligned}\Psi_i^{(1)} &= |0, 0, \dots, n_i = 1, 0, 0, \dots\rangle \\ &= |\mu_i\rangle.\end{aligned}$$

The one-particle states span the single-particle subspace of the linear vector space. The one-particle states, two-particle states, and the states for other numbers of particles, together with all of the linear combinations of all of these states, make up the linear vector space for a many-body system. This linear vector space is a Fock space (Merzbacher 1970:510). Fock space is a Hilbert space very suitable for use with systems containing an indefinite number of particles. In nonrelativistic many-body theory, the variable particle number can occur because of the transfer of particles across the boundaries of the system, rather than because of the creation or annihilation of particles (Mohling 1982:153).

## 5. Operator Hilbert Spaces

### 5.1. Superspaces

It can be useful even in nonrelativistic quantum field theory to consider generalized Hilbert spaces. The generalizations to be made will involve the nature of the elements in the space, the operators on the space, and the inner product.

It is possible to generalize the notion of a function space to that of an operator space. In particular, it is possible to conceive of an operator Hilbert space. Because such a space is a vector space, the elements can be called vectors, but these elements are operators rather than the functions of an ordinary Hilbert space. Because operators act on the elements of an ordinary Hilbert space, but are themselves merely elements in an operator Hilbert space, any example of the latter sort of space can be given the appellation "superspace". The mathematical entities that function as actual operators in a superspace by acting on the elements, which are ordinary operators, can likewise loosely be termed "superoperators". To complete the terminology, the ordinary operators that are the elements of the space can loosely be called "superspace vectors".

A separable operator Hilbert space is thus a superspace spanned by a countably infinite set of basis operators which are superspace vectors. An uncountably infinite set of

other operators, which are also superspace vectors, can be constructed in the space from linear combinations of multiples of the basis operators. Superoperators, which functionally are operators, map operators, which functionally are superspace vectors, onto operators in the space. Superoperators of physical interest preserve linearity of the space.

## 5.2. Fermi Space

A particular type of operator Hilbert space, designated as the associated Hilbert space, has been used in an attempt at field quantization (Crawford 1958). The elements of this superspace are linear combinations of products of odd numbers of second-quantized fermion stepping operators. Because of this, the space is sometimes called a Fermi space. It has been shown that such a space does indeed have the properties of a generalized abstract Hilbert space (Bowen 1975).

Because the associated Hilbert space is a superspace, its elements can be regarded as superspace vectors. Because the space is a Hilbert space, it has a scalar, or inner, product. The scalar product of two superspace vectors in the space is defined to be the thermal average of their anticommutator, calculated in the grand canonical ensemble. For this reason, the associated Hilbert space is called an anticommutator space. The use of the anticommutator is

appropriate to the antisymmetry of the wave function for fermions.

At this point some special notation is introduced, including the double parentheses for an inner product in an operator Hilbert space (Bowen 1975).

The scalar product of two superspace vectors  $\hat{A}$  and  $\hat{B}$  in Fermi space is thus defined to be

$$((\hat{A}, \hat{B}))_a = \langle \hat{B}, \hat{A}^+ \rangle.$$

### 5.3. Bose Space

Each kind of elementary particle can be assigned to one of two classes on the basis of the statistical properties of identical particles. Fermions, subject to the Pauli exclusion principle, obey Fermi-Dirac statistics, and are characterized in a first-quantized Schroedinger representation by antisymmetry of the wave function under exchange of any two fermions, and in a second-quantized Heisenberg representation by canonical anticommutation relations of stepping operators. As has been mentioned, the property that fermion operators are subject to anticommutation relations is used in the definition of an inner product in Fermi (anticommutator) space.

Particles belonging to the other class are called bosons. They are not subject to the Pauli exclusion principle, and therefore obey Bose-Einstein statistics.

They are characterized in a first-quantized Schroedinger representation by symmetry of the wave function under exchange, and in a second-quantized Heisenberg representation by canonical commutation relations of stepping operators.

All of these properties of bosons are an expression of the fact that there can be boson states in which two or more - in fact, very many - bosons of the same kind, and with the same quantum numbers, exist simultaneously. It is this fact, and the concomitant properties, that make interactions involving bosons so difficult to work with mathematically.

By analogy with Fermi space, it is possible to have a space determined by the commutation properties of bosons. Furthermore, it is useful to consider two kinds of commutator spaces. In Bose space, the scalar product of two superspace vectors is not defined to be simply the thermal average of their commutator in the grand canonical ensemble. It happens that symmetry considerations and the requirement that the scalar product be positive definite lead to a more complicated definition (Bowen 1975).

The scalar product of two superspace vectors  $\hat{A}$  and  $\hat{B}$  in Bose space is thus defined to be

$$((\hat{A}, \hat{B}))_b = \langle [[\hat{B}, \hat{H}], \hat{A}^+] \rangle.$$

If the requirement that the scalar product be positive

definite can be eliminated or ignored, it is possible to have a commutator space different from Bose space. What is called Pontryagin space is such as space.

#### 5.4. Pontryagin Space

Hilbert spaces have been defined to have non-negative norms, arising from inner products. Now it is necessary to consider the possibility of negative norms. Normed linear vector spaces that can have negative as well as positive norms are said to have an indefinite metric. A linear vector space with an indefinite metric is called a Krein space (Bognar 1974). A Hilbert space with an indefinite metric is called a Pontryagin space (Krein and Langer 1964). (Another reference is Langer, G. K. n.d. Lecture notes, unpublished, math. dept., Univ. Dresden, G.D.R.)

Let  $X$  be a normed linear vector space with an indefinite metric. A vector  $x \in X$  is characterized by an indefinite norm as follows:

$$(x, x) > 0 \Rightarrow \text{positive } x,$$

$$(x, x) = 0 \Rightarrow \text{neutral } x,$$

$$(x, x) < 0 \Rightarrow \text{negative } x.$$

A neutral vector in the vector space,

$$\{x : x \in X \ni (x, x) = 0 \vee x \neq 0\},$$

can be written as the sum of positive and negative vectors. It is not in the equivalency class of the null vector.

The value of using spaces with an indefinite metric in

efforts to get consistent quantization of fields has been recognized for some time (Dirac 1942; Pauli 1943). A well-known quantization of the electromagnetic field, in which a canonical quantization of all four components of the vector potential led to a manifestly covariant local theory, required a metric that was not positive definite (Bleuler 1950; Gupta 1950, 1962). Indefinite metrics soon appeared in attempts to "regularize" divergent integrals (Pauli and Villars 1949), in field theories with higher-order Lagrangians (Green 1948; Pais and Uhlenbeck 1950), and in explanations of "ghost states" in theories of elementary particles (Heisenberg 1957). Literature of the period referenced applications not only to the electromagnetic field, but also to the vector meson field and to the gravitational field (Nagy 1960, 1966, 1970). It also addressed concerns about whether or not an indefinite metric was consistent with the usual probabilistic interpretations (Arons et al. 1965) and with the desired unitarity of the scattering matrix (Lee and Wick 1969). The proper interpretation of the indefinite metric in relativistic quantum field theory is still a matter of controversy (Berger 1983).

A Pontryagin space that is a commutator space is the only space with an indefinite metric that will be of further interest here. The scalar product of two superspace vectors

in this space is defined to be the thermal average of their commutator, calculated in the grand canonical ensemble.

Then the space is clearly a commutator space.

The scalar product of two superspace vectors A and B in a commutator Pontryagin space is thus defined to be

$$((\hat{A}, \hat{B}))_c = \langle [\hat{B}, \hat{A}^+] \rangle.$$

The decision as to which of the two types of commutator space, Bose or Pontryagin, to use in a particular situation is usually made on the basis of expediency. The appropriate choice is suggested by the relative convenience or ease of calculation accruing from the use of one or the other method. For example, the normalization of a neutral vector is a problem in a commutator Pontryagin space because of the vanishing of the scalar product.

### 5.5. Density Operator

The density operator is an example of a neutral vector in a Pontryagin space. (This and subsequent references to a Pontryagin space will mean a commutator Pontryagin space.) In three-dimensional momentum space, the subscripts in the expression for the density operator would be the wave vectors  $\vec{k}$ ,  $\vec{q}$  and the like. For simplicity, the density operator and its adjoint are written for a single dimension:

$$\hat{P}_q = \sum_k \hat{c}_{k-q}^+ \hat{c}_k \neq 0,$$

$$\hat{P}_q^+ = \sum_k \hat{c}_k^+ \hat{c}_{k-q}.$$

The subscript appearing in the notation for a scalar product, indicating the space in which the scalar product is to be calculated, can often be omitted. If details of the calculation are shown, the nature of the space is evident from the form of the scalar product.

In Pontryagin space, the vanishing scalar product (inner product) of the density operator is

$$\begin{aligned} ((\hat{P}_q, \hat{P}_q)) &= \langle [\hat{P}_q, \hat{P}_q^+] \rangle = \langle \hat{P}_q \hat{P}_q^+ - \hat{P}_q^+ \hat{P}_q \rangle \\ &= \langle \sum_k \hat{c}_{k-q}^+ \hat{c}_k \sum_{k'} \hat{c}_{k'}^+ \hat{c}_{k'-q} \\ &\quad - \sum_{k'} \hat{c}_{k'}^+ \hat{c}_{k'-q} \sum_k \hat{c}_{k-q}^+ \hat{c}_k \rangle \\ &= \langle \sum_k (\hat{c}_{k-q}^+ \hat{c}_{k-q} - \hat{c}_k^+ \hat{c}_k) \rangle \\ &= \sum_{k'} N_{k'} - \sum_k N_k \\ &= 0; \end{aligned}$$

$$\therefore \hat{P}_q \neq 0,$$

$$((\hat{P}_q, \hat{P}_q)) = 0.$$

### 5.6. Conditional Operators

It has been shown that Bose, Fermi and Pontryagin spaces are characterized by the commutation or anticommutation relations of the elements of the spaces. It thus has also been suggested that the elements of these spaces could be products of second-quantized stepping operators. An explanation of stepping operators can be found in discussions of identical particles in quantum mechanics (Merzbacher 1970).

The commutation relations for stepping operators for bosons are these:

$$\hat{a}_m^+ \hat{a}_n^+ - \hat{a}_n^+ \hat{a}_m^+ = 0,$$

$$\hat{a}_m \hat{a}_n - \hat{a}_n \hat{a}_m = 0,$$

$$\hat{a}_m \hat{a}_n^+ - \hat{a}_n^+ \hat{a}_m = \delta_{mn}.$$

The anticommutation relations for stepping operators for fermions are these:

$$\hat{b}_m^+ \hat{b}_n^+ + \hat{b}_n^+ \hat{b}_m^+ = 0,$$

$$\hat{b}_m \hat{b}_n + \hat{b}_n \hat{b}_m = 0,$$

$$\hat{b}_m \hat{b}_n^+ + \hat{b}_n^+ \hat{b}_m = \delta_{mn}.$$

Stepping operators symbolize changes in the number of particles in a system; a single creation operator symbolizes an addition of a particle, whereas a single

annihilation operator symbolizes the subtraction of a particle from the system. Products of an odd or even number of stepping operators can symbolize a corresponding odd or even change in the number of particles in the system. Such products compose the elements of a Bose or Fermi space. A comparison of symmetry properties of the commutation (or anticommutation) properties of boson and fermion stepping operators with the commutation (or anticommutation) properties of a Bose, Fermi or Pontryagin spaces shows that if elements of the space symbolize an odd change in the number of fermions, the space is a Fermi space, but if the elements of the space symbolize an even change in the number of fermions or either an odd or even change in the number of bosons, the space is a Bose space or a Pontryagin space.

A superspace vector can be expanded in terms of a chosen basis set in an operator Hilbert space. The basis is chosen to be an orthonormal set of linearly independent second-quantized operators. It is useful to choose the second-quantized operators to be conditional stepping operators. A conditional stepping operator might be, for example, an operator that creates elementary excitations in particular states only when certain other physical requirements are simultaneously satisfied. If elementary excitations can be decomposed into linear combinations of conditional operators, the nature of corresponding physical

processes can be determined (Bowen et al. 1984).

For instance, consider a decomposition of

$$\hat{\phi}_{ij} = \hat{X}_i \hat{Y}_j$$

where  $\hat{X}_i$  and  $\hat{Y}_j$  are fermion and boson factors, respectively.

Suppose that two different kinds of fermions are involved.

Then the fermion factor might be decomposed into these conditional operators:

$$\hat{b}^+ \hat{b} \hat{c},$$

$$\hat{c}^+ \hat{c} \hat{b},$$

$$(1 - \hat{b}^+ \hat{b}) \hat{c},$$

$$(1 - \hat{c}^+ \hat{c}) \hat{b}.$$

The conditional nature of these operators is evident. The operator  $\hat{b}^+ \hat{b} \hat{c}$ , for example, annihilates a  $\hat{c}$ -type fermion only if a  $\hat{b}$ -type fermion exists ( $\hat{b}^+ \hat{b} = 1$ ). On the other hand, the operator  $(1 - \hat{b}^+ \hat{b}) \hat{c}$  annihilates a  $\hat{c}$ -type fermion only if there is no  $\hat{b}$ -type fermion ( $\hat{b}^+ \hat{b} = 0$ ). The other pair of operators is similar in these respects.

Simple relationships such as the following can be found among these conditional operators:

$$(1 - \hat{b}^+ \hat{b}) \hat{c} + \hat{b}^+ \hat{b} \hat{c} = \hat{c}.$$

The fermion factor has been decomposed into simple conditional operators. The boson factor is not so easily handled. Indeed, it turns out to be possible to guess that

it should decompose into conditional operators of the forms

$$\hat{a}^n \hat{I}_n(\lambda/\omega),$$

$$\hat{I}_n(\lambda/\omega) (\hat{a}^\dagger)^n,$$

that have interrelationships resembling

$$\hat{J}_0(\lambda/\omega) + \sum_k [\hat{a}^k \hat{I}_k(\lambda/\omega) + \hat{I}_k(\lambda/\omega) (\hat{a}^\dagger)^k] = I,$$

where the  $\hat{I}_n(\lambda/\omega)$  and  $\hat{J}_0(\lambda/\omega)$  terms involve powers of  $\hat{a}^\dagger \hat{a}$  and where the proliferation of boson stepping operators is very evident. A detailed scrutiny of this problem constitutes a considerable portion of what remains to be discussed.

The conditional stepping operators belong to an algebra of operators. This algebra is often a Lie algebra.

## 6. Application of Lie Groups

### 6.1. Algebra

The discussion now returns to a further consideration of algebraic structures, beginning with the definition of a ring. A ring  $R$  is an additive Abelian group, the elements of which can not only be added, but can also be combined by the operation of multiplication to form a product  $c = a \cdot b$ . The operation of multiplication has the following properties:

(1) It is closed:

$$\forall a, b \in R \exists a \cdot b = c \in R.$$

(2) It is associative:

$$(\forall a, b, c \in R)[a \cdot (b \cdot c) = (a \cdot b) \cdot c].$$

(3) It is distributive:

$$\begin{aligned} (\forall a, b, c \in R)[a \cdot (b + c) &= a \cdot b + a \cdot c], \\ \forall [(a + b) \cdot c &= a \cdot c + b \cdot c]. \end{aligned}$$

The elements in a ring can be multiplied by each other, according to the operation of multiplication. If the operation of multiplication is also commutative, the ring is called a commutative ring. If the operation of multiplication is not associative, the ring is a nonassociative ring (Herstein 1964).

An algebra  $A$  is a linear vector space in which the vector can be multiplied in such a way that the linear vector space is also a ring in which multiplication by

scalars and multiplication are related by

$$\alpha(a \cdot b) = (\alpha a) \cdot b = a \cdot (\alpha b).$$

An ideal in an algebra  $A$  is a subset  $I$  characterized by three properties:

- (1)  $I$  is a linear subspace of  $A$ ,
- (2)  $i \in I \Rightarrow ai \in I \forall a \in A$ ,
- (3)  $i \in I \Rightarrow ia \in I \forall a \in A$ .

If  $I$  satisfies only the first two of these three conditions, it is a left ideal.

If  $I$  is a proper subset of  $A$ , then  $I$  is contained in but not equal to  $A$ , and is called a proper ideal. The relation is written  $I \subset A$ .

A maximal left ideal is a proper left ideal that is not properly contained in any other proper left ideal.

An algebra  $A$  is semi-simple if every non-zero element of  $A$  is outside some maximal left ideal. A semi-simple algebra is an algebra with no Abelian ideals (Gilmore 1974).

## 6.2. Lie Algebra

Lie algebras are related to a number of concepts that have connections with the Liouville resolvent method. They are associated with conditional stepping operators and with the most important operator to be discussed, the Liouville operator. They are also associated with canonical transformations. They are even associated with Bessel functions (Miller 1968; Talman 1968:199-202),

generalizations of which will be discussed. Because of this, a summary of relevant background material is given here. The summary begins with the definition of a group (Herstein 1964; Burington 1965).

As has been mentioned, a Hilbert space is a particular kind of linear vector space, and a linear vector space is a particular kind of group. The order of a finite group is the number of elements in the group. An infinite group has an infinite number of elements. An infinite-dimensional Hilbert space is a particular kind of infinite group. The elements of a continuous group, unlike those of a discrete group, are functions of real parameters that are continuously variable.

Consider an  $n$ -parameter infinite group (Mathews and Walker 1970). Elements are labeled by  $n$  real parameters that vary continuously:

$$g(x) = g(x_1, x_2, \dots, x_n).$$

Define the product of elements:

$$\begin{aligned} g(x_1, x_2, \dots, x_n)g(y_1, y_2, \dots, y_n) \\ = g(z_1, z_2, \dots, z_n). \end{aligned}$$

Get a table of  $n$  real functions, each with  $n$  real arguments:

$$z_1 = f_1(x_1, \dots, x_n, y_1, \dots, y_n),$$

...

$$z_n = f_n(x_1, \dots, x_n, y_1, \dots, y_n),$$

The group is a Lie group if the  $f_i(x, y)$  have these properties:

- (1) they satisfy group properties,
- (2) they are continuous,
- (3) they have derivatives of all orders.

Define the identity element of the group:

$$g(0) = g(0, 0, \dots, 0),$$

$$g(0)g(x) = g(x).$$

If every element of a group can be represented as a finite product in terms of a set of independent elements of the group, the set of independent elements is a set of independent generators of the group. For each parameter of the Lie group there is a generator:

$$x_1 = \lim_{\epsilon \rightarrow 0} \frac{g(a, 0, \dots, 0) - g(0, 0, \dots, 0)}{\epsilon},$$

$$x_2 = \lim_{\epsilon \rightarrow 0} \frac{g(0, \epsilon, \dots, 0) - g(0, 0, \dots, 0)}{\epsilon},$$

...

$$x_n = \lim_{\epsilon \rightarrow 0} \frac{g(0, 0, \dots, \epsilon) - g(0, 0, \dots, 0)}{\epsilon}.$$

The Lie algebra associated with the Lie group is composed of all linear combinations of generators with real coefficients  $c_n$ :

$$c_1 x_1 + c_2 x_2 + \dots + c_n x_n.$$

This satisfies the definition of an algebra if the product of two elements is their commutator.

The second-quantized stepping operators can be related to Lie algebras (Georgi 1981).

The phase space of operators is the  $(2n)$ -dimensional space defined at time  $t$  by the set of stepping operators

$$z = (\hat{a}_1(t), \dots, \hat{a}_n(t), \hat{a}_1^\dagger(t), \dots, \hat{a}_n^\dagger(t)).$$

The bracket

$$[\hat{a}_i, \hat{a}_i^\dagger] = 1, \quad i = 1, n$$

is a commutator for boson operators and an anticommutator for fermion operators.

An analog to the classical Poisson bracket is

$$[z_i, z_j] = J_{ij}, \quad i, j = 1, \dots, 2n$$

$$= \begin{bmatrix} 0 & I \\ \pm I & 0 \end{bmatrix}.$$

The  $I$  is an identity matrix; the plus sign is appropriate for fermions, the minus sign for bosons.

The state space is the  $(2n + 1)$ -dimensional space defined by the set  $\{z, t\}$ .

The analytic function space  $F$  is the space generated by all of those functions on state space that can be expanded as follows:

$$f(z) = \sum_{\{n_i\}} c_{\{n_i\}} z^{\{n_i\}},$$

$$z^{\{n_i\}} = \left[ [z_{2n}]^{n_{2n}} \right] \left[ [z_{2n-1}]^{n_{2n-1}} \right] \dots \left[ [z_1]^{n_1} \right],$$

$$n_i \geq 0.$$

The analytic functions of  $F$  form a Lie algebra.

The Lie operator  $L_f$  is a representation  $\rho(f)$  of a Lie algebra  $F$ .

The Lie operator  $L_f$  generated by a function  $f \in F$  acting on  $F$  is defined by the commutator

$$L_f g = [g, f], \quad g \in F.$$

The negative of a Lie operator is sometimes called an adjoint operator. The Lie operators form a Lie algebra under commutation that is homomorphic to the Lie algebra of analytic functions on  $F$ .

The Lie series is the series

$$\sum_{n=0}^{\infty} c_n L_f^n.$$

The Lie transformation is the particular Lie series given by

$$\exp(L_f) \equiv \sum_{n=0}^{\infty} \frac{1}{n!} L_f^n.$$

A Lie transformation  $\exp(L_f)$  is a canonical

transformation subject to the condition

$$f^* = -f.$$

A Lie product on  $F$  is the commutator

$$P(f, g) = [f, g] \quad \forall f, g \in F.$$

It is a Lie algebra.

### 6.3. Cartan Subalgebra

Consider a Lie algebra  $A$  on a vector space  $V$ .

A representation  $\rho$  of  $A$  on  $V$  is a mapping that assigns a linear transformation  $\rho(\lambda)$  on  $V \quad \forall \lambda \in A$ ,  $\exists$

$$\rho(\alpha\lambda + \beta\mu) = \alpha\rho(\lambda) + \beta\rho(\mu),$$

$$\rho[\lambda, \mu] = [\rho(\lambda), \rho(\mu)].$$

A linear functional  $\alpha$  on  $A$  is a weight of  $\rho$  if  $\exists$  a non-zero vector  $v \in V \ni$

$$\rho(\lambda)v = \alpha(\lambda)v \quad \forall \lambda \in A.$$

Then  $v$  is a weight vector belonging to  $\alpha$ .

A vector  $v$  is a generalized weight vector belonging to a weight  $\alpha$  if  $\exists$  an integer  $n$  large enough so that

$$[\rho(\lambda) - \alpha(\lambda)I]^n v = 0 \quad \forall \lambda \in A.$$

The linear space of all generalized weight vectors belonging to the weight  $\alpha$  is the weight space  $V_\alpha$  of  $\rho$  belonging to  $\alpha$ .

A Lie algebra  $A$  is nilpotent if  $A^n = 0$  for large enough  $n$ .

Consider a complex Lie algebra  $A$  and a nilpotent subalgebra  $M$ . The mapping  $M \rightarrow \text{adjoint } M$  is the adjoint

representation of  $M$  on  $A$ . The weights  $\alpha$  are the roots on  $M$  and the weight space  $V_\alpha$  is the root space.

If the root space corresponding to the root  $\theta$  of  $M$  is  $A_0$ , then  $M$  is a Cartan subalgebra if  $M = A_0$ .

#### 6.4. Group $U(n)$

Conditional stepping operators belong to an algebra of operators. This algebra is usually considered to be some large Lie algebra of unitary type  $U(n)$  for some large  $n$  (Judd and Elliott 1970:21-25).

Although the overall structure of the algebra does not appear to provide clues for the efficient construction of conditional operators to be used for calculations, some of the properties of the algebra can be useful.

A group can be represented by a square matrix. The group  $U(n)$  can be represented by  $n \times n$  unitary matrices. The generators of  $U(n)$  are  $n^2 - 1$  traceless  $n \times n$  Hermitian matrices and an  $n \times n$  unitary matrix  $I_n$ . The one-dimensional Abelian subspace spanned by  $I_n$  is an ideal. The subspace of the traceless  $n \times n$  Hermitian matrices on a real field is an ideal, not necessarily Abelian. (A reference is Que, W. 1984. Research notes, unpublished. Phys. dept. Va. Tech.)

Two types of operators in  $U(n)$  are the following:

- (1) orthogonal projection operators  $\hat{H}_1$ ,
- (2) Judd shift operators  $\hat{\phi}_\alpha$ .

The orthogonal projection operators  $\hat{H}_i$  commute among themselves. The maximal Cartan subalgebra is the largest set of these. A representation of the algebra in the maximal Cartan form is the representation with the most selectivity. This selectivity makes it easier to diagonalize operators (Wan 1975). Properties of commutation or anticommutation relations for the canonical Cartan form of a Lie algebra make some symmetry consideration and some calculations easier.

The remaining elements of the Lie algebra are the Judd shift operators  $\hat{\phi}_\alpha$ , which are the conditional stepping operators.

In standard Lie algebra, labels for the stepping operators are formed from the root vectors, which are n-tuples  $\alpha$  containing the eigenvalues  $\alpha_\lambda$  of  $\hat{\phi}_\alpha$  in commutation with the  $i$ th orthogonal projection operator  $\hat{H}_i$ . This commutation relation, along with three others, comprise the essential structure of the Lie algebra. These canonical commutation relations show an isomorphism between semi-simple algebras of rank  $n$  and sets of roots in  $n$ -dimensional  $R_n$ :

$$[\hat{H}_i, \hat{\phi}_\alpha] = a_i \hat{\phi}_\alpha,$$

$$[\hat{H}_i, \hat{H}_j] = 0,$$

$$[\hat{\phi}_\alpha, \hat{\phi}_\alpha^\dagger] = \sum_{i=1}^n \alpha_i \hat{H}_i,$$

$$[\hat{\phi}_\alpha, \hat{\phi}_\beta] = N_{\alpha\beta}^\gamma \hat{\phi}_\gamma.$$

The  $N_{\alpha\beta}^\gamma$  are remaining non-zero structure constants for the group.

### 6.5. Judd Procedure

The Judd procedure constructs the Cartan form of the Lie algebra directly (Judd 1962).

Expand a single-particle stepping operator (for either fermions or bosons) by

$$\hat{c} = \sum_i b_i \hat{\psi}_i,$$

where the coefficients  $b_i$  involve thermal averages arising from normalization of the  $\hat{\psi}$  in superspace, and where the  $\hat{\psi}_i$  are linear combinations of Judd operators  $\hat{\phi}_\alpha$ . The single-particle stepping operator is thus expanded in terms of the Judd operators.

Express a given physical state  $|\hat{\Psi}\rangle$  in Fock space as a product of second-quantized creation operators, in some canonical ordering, acting on the vacuum state  $|0\rangle$ :

$$\begin{aligned} |\hat{\Psi}\rangle &= \hat{c}_1^\dagger \hat{c}_2^\dagger \dots \hat{c}_n^\dagger |0\rangle \\ &= \hat{A}_n^\dagger |0\rangle \end{aligned}$$

with

$$\hat{A}_n = \hat{c}_n \hat{c}_{n-1} \cdots \hat{c}_2 \hat{c}_1.$$

Define an operator  $\hat{A}_\theta^\dagger$  that creates a filled set of states.

The invariant idempotent projection operator for an empty set of states, or the vacuum state, is

$$\hat{I}_\theta = \hat{A}_\theta \hat{A}_\theta^\dagger.$$

Construct the Judd operator

$$\hat{\Phi} = \hat{A}_n^\dagger \hat{I}_\theta \hat{A}_m.$$

The Judd operator is a stepping operator for  $m \neq n$ . It annihilates a configuration with  $\hat{A}_m$ , and creates a new configuration with  $\hat{A}_n^\dagger$ . In condensed-matter physics, the Judd operators are many-particle stepping operators that allow a stepping between a state with  $m$  particles and a state with  $n$  particles.

Let  $|\hat{\Psi}(n)\rangle$  and  $|\hat{\Psi}'(n')\rangle$  be sets of states of  $n$  and  $n'$  particles respectively for a system. The Lie algebra associated with the system and its states is made up of the set of operators

$$\hat{\Phi}_{nn'} = \hat{A}_{\Psi(n)}^\dagger \hat{I}_\theta \hat{A}_{\Psi'(n')}.$$

For  $n - n' = 1$  this is the particular set of operators that annihilates one particle, and is the class of one-particle conditional annihilation operators that can be used to construct the one-electron Green function for many-particle systems.

Several possible advantages can follow from the use of Judd operators:

- (1) Exact solutions can be obtained for simple many-body problems.
- (2) Mean-field approximations can be surpassed.
- (3) Scalar products in superspace can be calculated with relative ease.
- (4) Canonical commutation relations for the Lie algebra are automatically obtained.
- (5) The Judd form of stepping operators can directly describe initial and final many-particle states.
- (6) With the aid of the basic commutation or anticommutation relations between one-particle stepping operators operating on a set of states, the Judd operators can be collapsed into a form that can often make the nature of conditional events more readily apparent.

The use of the Judd procedure to calculate conditional stepping operators for states of electrons in an atomic shell is a simple instructive example that is described in the literature (Bowen et al. 1984).

## 7. Liouville Resolvent Method

### 7.1. Green Functions

Green functions are widely used because they contain in an economical and generally extractable form all of the information that is usually of interest regarding a physical system.

In classical mechanics, the response of a physical system to linear perturbations can be expressed in terms of a Green function that is independent of the perturbation. The Green function is a solution to a differential equation modeling the response. Boundary conditions determine the exact form of the Green function, and so are implicitly included in the Green function.

In quantum field theory, non-linear Green functions can be used. In any case, the Green function determines the thermodynamic potential and therefore the thermodynamic properties, including the density of states in energy, of a many-particle system. In principle, then, all of the information of interest about a system can be obtained from the Green function, without the necessity of finding eigenstates and energy eigenvalues by solving an equation such as

$$i\hbar \frac{\partial \hat{\rho}}{\partial t} = [\hat{H}_0 + \hat{H}', \hat{\rho}].$$

A single-particle Green function describes what happens

when an extra particle is added to a many-particle system. In many-body theory it is often assumed that the number of particles  $N$  in the system can vary but that the chemical potential  $\mu$  is fixed. The chemical potential (March et al. 1967; Pathria 1972; Mohling 1982) is related to the energy involved in adding a particle to the system. Because the number of particles in the system can vary, the grand canonical ensemble is used. The thermodynamic potential is

$$\Omega = -kT \ln Z,$$

expressed in terms of the grand partition function,

$$Z = \text{Tr} \exp[-\beta(\hat{H} - \mu\hat{N})],$$

$$\beta = 1/kT.$$

A double-time Green function, whether a retarded Green function, an advanced Green function, a causal Green function for zero temperature, or a temperature Green function for finite temperature, describes the propagation of a particle between one time and another (Rickayzen 1980).

A double-time Green function is actually a function of the difference between two times, reflecting translational invariance in time.

A Green function can be Fourier-transformed for various purposes. For example, the energy and lifetime of a particle in interaction with other parts of the system can in principle be found from the pole or poles, in the complex

$\epsilon$  plane, of the transformed function,

$$G_{\vec{k}}(\omega) = \int_{-\infty}^{\infty} e^{i\omega t} G_{\vec{k}}(t) dt.$$

For a Green function of the form

$$G_{\vec{k}}(t) = -ic_{\vec{k}} e^{-i\hbar\omega_{I,\vec{k}}t - \delta t},$$

the transformed function is

$$G_{\vec{k}}(\omega + i\delta) = c_{\vec{k}} \frac{1}{\omega - \omega_{\vec{k}} + i\delta},$$

where  $\delta$  is the reciprocal lifetime of the particle and the subscripted  $\omega$  is the energy (Haken 1976). Define a subscripted bracket as

$$[\hat{A}, \hat{B}]_{\eta} = \hat{A}\hat{B} + \eta\hat{B}\hat{A}.$$

A commutator can be written as

$$\begin{aligned} [\hat{A}, \hat{B}]_{\eta=-1} &= [\hat{A}, \hat{B}]_{-} \\ &= [\hat{A}, \hat{B}] \\ &= \hat{A}\hat{B} - \hat{B}\hat{A}. \end{aligned}$$

An anticommutator can be written as

$$\begin{aligned} [\hat{A}, \hat{B}]_{\eta=+1} &= [\hat{A}, \hat{B}]_{+} \\ &= \{\hat{A}, \hat{B}\} \\ &= \hat{A}\hat{B} + \hat{B}\hat{A}. \end{aligned}$$

A retarded Green function describes what is called in

classical mechanics the admittance of a system. With the use of the unit step function  $\theta(t)$ , the retarded Green function for two operators  $\hat{A}$  and  $\hat{B}$  can be written as

$$\begin{aligned} G_R(t, t') &= G_R(t - t') \\ &= -i/\hbar \langle [\hat{A}(t), \hat{B}(t')]_{\eta} \rangle \theta(t - t'). \end{aligned}$$

It is conventional to work with a system of units in which  $\hbar$  has unit value. In accordance with this convention, the  $\hbar$  is ordinarily "dropped" from the expression for the Green function unless dimensional relationships are to be emphasized. This convention will be followed in the subsequent discussions.

The time Fourier transform of a retarded Green function describes the response of a system to a sinusoidal force of some angular frequency  $\omega$ . For a complex

$$z = \omega + i\delta$$

it is defined by

$$G_R(\omega) = \lim_{\delta \rightarrow 0} G_R(z),$$

where

$$G_R(z) = \int_{-\infty}^{\infty} dt \exp[iz(t - t')] G_R(t - t').$$

For the  $G_R(t - t')$  for two operators  $\hat{A}$  and  $\hat{B}$ , this last expression is

$$\begin{aligned}
G_R(z) &= -i \int_{-\infty}^{\infty} dt \exp[iz(t - t')] \\
&\quad \times \langle [\hat{A}(t), \hat{B}(t')]_{\eta} \rangle \theta(t - t') \\
&= -i \int_0^{\infty} dt \exp(izt) \langle [\hat{A}(t), \hat{B}(0)]_{\eta} \rangle.
\end{aligned}$$

The  $G(t, t')$  is a function of the time difference only, as a manifestation of translational invariance in time. For convenience, therefore, the time scale can be shifted arbitrarily so that  $t'$  is zero.

Inner products over an operator Hilbert space have been defined in such a way that they can be written as

$$((\hat{B}, \hat{A})) = \langle [\hat{L}^s \hat{A}, \hat{B}^\dagger]_{\eta} \rangle,$$

where

$$\begin{aligned}
s &= 0 \text{ for Fermi or Pontryagin space} \\
&= 1 \text{ for Bose space,}
\end{aligned}$$

and where

$$\begin{aligned}
\eta &= -1 \text{ for Fermi space} \\
&= +1 \text{ for Bose or Pontryagin space.}
\end{aligned}$$

The thermal average of an operator  $\hat{C}$  is denoted by

$$\langle \hat{C} \rangle = \text{Tr}(\rho \hat{C}).$$

A scalar product over an abstract Hilbert space has been defined to be a thermal average and is therefore a function of a density matrix  $\rho$ . These properties are implicitly indicated by the double parentheses.

With some further special notation (Zubarev 1960), the retarded thermodynamic Green function for two conditional second-quantized stepping operators  $\hat{A}$  and  $\hat{B}^+$  can be written as

$$\begin{aligned}
 G(t,0) &= G(t - 0) \\
 &= G(t) \\
 &= \langle\langle \hat{A}; \hat{B}^+ \rangle\rangle_t \\
 &= \langle\langle \hat{A}(t); \hat{B}^+(0) \rangle\rangle \\
 &= -\eta \theta(t) \langle [\hat{A}(t), \hat{B}^+(0)] \rangle. \quad \eta
 \end{aligned}$$

When  $\eta$  is minus one, the conditional operators  $\hat{A}$  and  $\hat{B}$  are products of an odd number of fermion stepping operators. The Green function has the written form

$$\langle\langle \hat{A}(t); \hat{B}^+(0) \rangle\rangle = -i\theta(t) \langle \{\hat{A}(t), \hat{B}^+(0)\} \rangle.$$

An example of a single-particle Green function of this kind is

$$\begin{aligned}
 G(\vec{k}, t) &= \langle\langle \hat{c}_{\vec{k}}(t); \hat{c}_{\vec{k}}^+(0) \rangle\rangle \\
 &= -i\theta(t) \langle \{\hat{c}_{\vec{k}}(t), \hat{c}_{\vec{k}}^+(0)\} \rangle.
 \end{aligned}$$

When  $\eta$  is one, there are two possibilities. For either possibility, the Green function has the written form

$$\langle\langle \hat{A}(t); \hat{B}^+(0) \rangle\rangle = -\theta(t) \langle [\hat{A}(t), \hat{B}^+(0)] \rangle.$$

When  $\eta$  is one, the first possibility is that the

conditional operators  $\hat{A}$  and  $\hat{B}$  are products of an even number of fermion stepping operators. An example of this kind of Green function is the density-density correlation function

$$\chi(\vec{q}, \omega) = -\theta(t) \langle [\hat{\rho}_{\vec{q}}(t), \hat{\rho}_{\vec{q}}^*(0)] \rangle,$$

with

$$\hat{\rho}_{\vec{q}} = \sum_{\vec{k}} \hat{c}_{\vec{k}}^{\dagger} \hat{c}_{\vec{k}-\vec{q}}.$$

For operators of the kind used here, it is convenient that the following condition holds:

$$[\hat{A}, \hat{A}^*] = 0.$$

It has already been shown, in the discussion of neutral vectors in Pontryagin space, that this condition is satisfied by  $\hat{\rho}_{\vec{q}}$ .

When  $\eta$  is one, the other possibility is that the conditional operators  $\hat{A}$  and  $\hat{B}$  are products of boson stepping operators. A representative Green function is

$$G(\vec{q}, t) = -\theta(t) \langle [\hat{a}_{\vec{q}}, \hat{a}_{\vec{q}}^*] \rangle.$$

## 7.2. Liouville Operator

The Poisson bracket (Goldstein 1980:397) of two variables  $u$  and  $v$  with respect to generalized coordinates and momenta  $q_j$  and  $p_j$  can be written, using a double-bracket notation, as

$$[[u, v]] = \sum_j \left[ \frac{\partial u}{\partial p_j} \frac{\partial v}{\partial q_j} - \frac{\partial u}{\partial q_j} \frac{\partial v}{\partial p_j} \right].$$

In classical mechanics, the Liouville operator  
(Killingbeck and Cole 1971:533)

$$L = -i \sum_j \left[ \frac{\partial H}{\partial p_j} \frac{\partial}{\partial q_j} - \frac{\partial H}{\partial q_j} \frac{\partial}{\partial p_j} \right]$$

acting on a variable  $u$  can be written in terms of a Poisson bracket as

$$Lu = i[[u, H]].$$

A Poisson bracket can be related to the commutator of two quantum-mechanical operators  $\hat{u}$  and  $\hat{v}$  (Merzbacher 1970:340) by the equations

$$\begin{aligned} [[u, v]] &= \lim_{\hbar \rightarrow 0} \frac{\langle [\hat{u}, \hat{v}] \rangle}{i\hbar} \\ &= \lim_{\hbar \rightarrow 0} \frac{[\hat{u}, \hat{v}]}{i\hbar}. \end{aligned}$$

Then

$$Lu = i \lim_{\hbar \rightarrow 0} \frac{\langle [\hat{u}, \hat{H}] \rangle}{i\hbar}.$$

The correspondence principle (Merzbacher 1970:338) requires a relation of the form

$$Lu = \lim_{\hbar \rightarrow 0} \langle \hat{L}\hat{u} \rangle,$$

involving the introduction of a quantum-mechanical Liouville

operator  $\hat{L}$ .

Then

$$\hat{L}\hat{u} = \frac{[\hat{u}, \hat{H}]}{\hbar}.$$

If  $\hbar$  has the value unity, then

$$\hat{L}\hat{u} = [\hat{u}, \hat{H}]. \quad (7.1)$$

The quantum-mechanical Liouville operator is a "superoperator", and can be called the Liouville superoperator. It is the quantum-mechanical analog of the classical Liouville operator.

A Lie operator  $L_f$  has been defined by the relation

$$L_f g = [g, f].$$

The superoperator  $\hat{L}$  fits the definition of a Lie operator. Superoperators in general are so-called adjoint operators on a Lie algebra.

The time-dependent operator

$$\hat{u}(t) = e^{-i\hat{L}t/\hbar}\hat{u}(0) \quad (7.2)$$

has the time derivative

$$\frac{\partial}{\partial t} \hat{u}(t) = -i \frac{\hat{L}}{\hbar} e^{-i\hat{L}t/\hbar}\hat{u}(0). \quad (7.3)$$

Substitution from Eq. (7.2) into Eq. (7.3) gives

$$\frac{\partial}{\partial t} \hat{u}(t) = -i \frac{\hat{L}}{\hbar} \hat{u}(t)$$

or

$$i\hbar \frac{\partial}{\partial t} \hat{\mu}(t) = \hat{L}\hat{\mu}(t). \quad (7.4)$$

Substitution from Eq. (7.1) into Eq. (7.4) gives (cf. Snygg 1981)

$$i\hbar \frac{\partial}{\partial t} \hat{\mu}(t) = [\hat{\mu}(t), \hat{H}]. \quad (7.5)$$

Taking the thermodynamic average of both sides of Eq. (7.5) leads to the equation

$$\frac{\partial}{\partial t} \langle \hat{\mu}(t) \rangle = \frac{\langle [\hat{\mu}(t), \hat{H}] \rangle}{i\hbar}.$$

The expression given by Eq. (7.2) for the time dependence of an operator may be compared with the conventional expression used in the Heisenberg representation of quantum mechanics:

$$\hat{\mu}(t) = e^{-i\hat{H}t/\hbar} \hat{\mu}(0) e^{i\hat{H}t/\hbar}.$$

### 7.3. Moment Expansion of Green Function

It is possible to use the Liouville superoperator to obtain a moment expansion of the Fourier transform of a single-particle Green function (Lonke 1971). A convenient example is the single-particle fermion Green function

$$\begin{aligned} G(t) &= \langle\langle \hat{c}(t); \hat{c}^+(0) \rangle\rangle \\ &= -i\theta(t) \langle\langle \hat{c}(t), \hat{c}^+(0) \rangle\rangle. \end{aligned} \quad (7.6)$$

The Heisenberg equation of motion for Eq. (7.6) is

$$i \frac{dG(t)}{dt} = i \frac{d}{dt} \langle\langle \hat{c}(t); \hat{c}^+(0) \rangle\rangle$$

$$\begin{aligned}
&= \delta(t) \langle \hat{c}(t), \hat{c}^+(0) \rangle \\
&\quad + \langle \langle [\hat{c}, \hat{H}]; \hat{c}^+ \rangle \rangle_t.
\end{aligned} \tag{7.7}$$

The commutator in Eq. (7.7) can be expressed in terms of the Liouville superoperator by means of the relation

$$\hat{L}\hat{c} = [\hat{c}, \hat{H}] \tag{7.8}$$

Substitution of Eq. (7.8) into Eq. (7.7) gives

$$\begin{aligned}
i \frac{d}{dt} \langle \hat{c}(t); \hat{c}^+(0) \rangle &= \delta(t) \langle \hat{c}(t), \hat{c}^+(0) \rangle \\
&\quad + \langle \langle \hat{L}\hat{c}; \hat{c}^+ \rangle \rangle_t.
\end{aligned} \tag{7.9}$$

The Fourier transform of Eq. (7.9) is

$$\omega \langle \langle \hat{c}; \hat{c}^+ \rangle \rangle_\omega = \langle \langle \hat{c}, \hat{c}^+ \rangle \rangle + \langle \langle \hat{L}\hat{c}; \hat{c}^+ \rangle \rangle_\omega. \tag{7.10}$$

Substituting  $\hat{c} \rightarrow \hat{L}\hat{c}$  into Eq. (7.10) gives

$$\omega \langle \langle \hat{L}\hat{c}; \hat{c}^+ \rangle \rangle_\omega = \langle \langle \hat{L}\hat{c}, \hat{c}^+ \rangle \rangle + \langle \langle \hat{L}^2\hat{c}; \hat{c}^+ \rangle \rangle_\omega. \tag{7.11}$$

Operation with  $\hat{L}$  on Eq. (7.8) shows the meaning of

$$\hat{L}^2\hat{c} = [[\hat{c}, \hat{H}], \hat{H}].$$

Substitution of Eq. (7.11) into Eq. (7.10) and division by  $\omega$  gives

$$\begin{aligned}
\langle \langle \hat{c}; \hat{c}^+ \rangle \rangle_\omega &= \omega^{-1} \langle \langle \hat{c}, \hat{c}^+ \rangle \rangle \\
&\quad + \omega^{-2} \langle \langle \hat{L}\hat{c}, \hat{c}^+ \rangle \rangle \\
&\quad + \omega^{-2} \langle \langle \hat{L}^2\hat{c}; \hat{c}^+ \rangle \rangle_\omega.
\end{aligned} \tag{7.12}$$

Next, a substitution of  $\hat{c} \rightarrow \hat{L}\hat{c}$  into Eq. (7.12), leading

to a repetition of the sort of procedure that began with the substitution of  $\hat{c} \rightarrow \hat{L}\hat{c}$  into Eq. (7.10), produces an expression containing a term involving  $\hat{L}^3\hat{c}$ . Continued iteration with this sort of procedure (Goldstein 1980) introduces higher and higher powers of the Liouville superoperator into the expression for the Fourier-transformed Green function, and generates the moment expansion

$$G(\omega) = \langle\langle \hat{c}; \hat{c}^+ \rangle\rangle_{\omega}$$

$$= \sum_{j=0}^{\infty} \frac{1}{\omega^{j+1}} \langle\langle \hat{L}^j \hat{c}, \hat{c}^+ \rangle\rangle. \quad (7.13)$$

Moment expansions can be generated for other functions, such as the density-density correlation function (Bowen 1975):

$$\chi(\vec{q}, \omega) = \sum_{j=0}^{\infty} \frac{1}{(\omega^2)^{j+1}} \langle\langle [\hat{L}^{2j+1} \hat{\rho}_{\vec{q}}, \hat{\rho}_{\vec{q}}^+] \rangle\rangle.$$

#### 7.4. Resolvent

A Green function can be equated to a matrix element of a resolvent of the Liouville superoperator by equating both to a moment expansion.

First, the resolvent of a matrix must be defined. (Bowen et al. 1984). If  $\underline{H}_N$  is an  $N \times N$  square Hermitian matrix,  $\underline{I}_N$  is the  $N \times N$  identity matrix, and  $z$  is a complex energy, then the secular matrix of  $\underline{H}_N$  is  $z\underline{I}_N - \underline{H}_N$ . The

vanishing of the determinant of the secular matrix constitutes the secular equation

$$|z\underline{I}_N - \underline{H}_N| = 0.$$

The real roots of the secular equation yield the eigenvalues of  $\underline{H}_N$ .

The matrix inverse of the secular matrix is the inverse operator or resolvent of  $\underline{H}_N$ ,

$$\underline{R}_N(z) = (z\underline{I}_N - \underline{H}_N)^{-1}.$$

The resolvent has poles on the real axis at eigenvalues of  $\underline{H}_N$ .

In the Heisenberg picture of quantum mechanics, a square matrix is often used to represent an operator. For example, a matrix  $\underline{H}_N$  could be used to represent a Hamiltonian operator  $\hat{H}$ . Then the resolvent of  $\underline{H}_N$ ,

$$\underline{R}_N(z) = (z\underline{I}_N - \underline{H}_N)^{-1},$$

could represent

$$\hat{R}(z) = (z\hat{I} - \hat{H})^{-1}.$$

The energy eigenvalues of  $\hat{H}_N$  would be on the real  $-z$  axis (where  $\delta$  is zero) and therefore would be zeros of the polynomial

$$|\omega\hat{I} - \hat{H}| = 0$$

or, equivalently, poles of the resolvent

$$\hat{R}(\omega) = (\omega\hat{I} - \hat{H})^{-1}.$$

The quantum-mechanical matrix elements of an operator represented in some orthogonal basis consisting of a set of basis functions  $\phi_n$  is

$$\hat{R}_{qn}(z) = \langle \phi_q | (z\hat{I} - \hat{H})^{-1} | \phi_n \rangle.$$

The matrix elements are analytic functions of  $z$  that approach zero in the manner of the inverse of  $z$  as the modulus of  $z$  approaches infinity away from the real axis. If the operator is Hermitian and has a continuous spectrum, the matrix elements have a branch cut on the real axis in the range of the continuous spectrum (Bowen et al. 1984).

It is ordinarily the case in quantum mechanics that the square matrices representing operators are infinite.

If the domain of the operator  $\hat{H}$  is an infinite-dimensional Hilbert space, then for all complex  $z$  farther than some small distance from the real axis, the matrix elements  $\hat{R}_{qn}(z)$ , of the resolvent of a finite  $N \times N$  square matrix  $\underline{H}_N$  representing a resolvent  $\hat{H}$ , converge to the exact result as  $N$  approaches infinity and the size of the matrix increases (Bowen et al. 1984).

### 7.5. Moment Expansion of Resolvent

A series analogous to a binomial series can be constructed for matrices or operators such as the resolvent

$$\begin{aligned}
\hat{R}(\omega) &= (\omega \hat{I} - \hat{H})^{-1} \\
&= \frac{1}{\omega} \left[ I - \frac{\hat{H}}{\omega} \right]^{-1} \\
&= \sum_{j=0}^{\infty} \frac{\hat{H}^j}{\omega^{j+1}} .
\end{aligned}$$

The matrix elements of the resolvent can be expressed in terms of the series as

$$\begin{aligned}
\langle \phi_q | (\omega \hat{I} - \hat{H})^{-1} | \phi_n \rangle \\
&= \langle \phi_q | \sum_{j=0}^{\infty} \frac{\hat{H}^j}{\omega^{j+1}} | \phi_n \rangle \\
&= \sum_{j=0}^{\infty} \frac{1}{\omega^{j+1}} \langle \phi_q | \hat{H}^j | \phi_n \rangle .
\end{aligned}$$

Similar expansions can be done for other sorts of resolvents, particularly those involving the Liouville superoperator. An important case will now be considered.

A Fermi inner product has been defined to have the form

$$\begin{aligned}
((\hat{B}, \hat{A})) &= \langle \hat{A}, \hat{B}^+ \rangle \\
&= \langle \hat{A} \hat{B}^+ \rangle + \langle \hat{B}^+ \hat{A} \rangle .
\end{aligned}$$

A resolvent of a Hermitian superoperator  $\hat{L}$ , such as the quantum-mechanical Liouville superoperator, is written as

$$\hat{R}(z) = (z \hat{I} - \hat{L})^{-1} .$$

If  $\hat{A}$  is replaced by  $\hat{R}(z)\hat{A}$  in the definition of the Fermi inner product, a special kind of matrix element of the

resolvent of  $\hat{L}$  can be defined that is the inner product

$$\begin{aligned}
 ((\hat{B}, \hat{R}(z)\hat{A})) &= ((\hat{B}, (z\hat{I} - \hat{L})^{-1}\hat{A})) \\
 &= \langle \{ (z\hat{I} - \hat{L})^{-1}\hat{A}, \hat{B}^+ \} \rangle \\
 &= \left\langle \left\{ \sum_{j=0}^{\infty} \frac{\hat{L}^j}{z^{j+1}} \hat{A}, \hat{B}^+ \right\} \right\rangle \\
 &= \sum_{j=0}^{\infty} \frac{1}{z^{j+1}} \langle \{ \hat{L}^j \hat{A}, \hat{B}^+ \} \rangle.
 \end{aligned}$$

Then

$$\begin{aligned}
 ((\hat{C}, (\omega\hat{I} - \hat{L})^{-1}\hat{C})) \\
 &= \sum_{j=0}^{\infty} \frac{1}{\omega^{j+1}} \langle \{ \hat{L}^j \hat{C}, \hat{C}^+ \} \rangle. \tag{7.14}
 \end{aligned}$$

A comparison of Eq. (7.14) with Eq. (7.13) demonstrates that the time Fourier-transformed Green function is an inner product that is a special kind of matrix element of the resolvent of the Hermitian superoperator  $\hat{L}$ . In general, for complex  $z$  and operators  $\hat{A}$  and  $\hat{B}^+$ , the equivalence is given by

$$\begin{aligned}
 G(z) &= \langle \langle \hat{A}; \hat{B}^+ \rangle \rangle_{\omega} \\
 &= \int_{-\infty}^{\infty} dt e^{izt} \langle \langle \hat{A}(t); \hat{B}^+(0) \rangle \rangle \\
 &= ((\hat{B}, (z\hat{I} - \hat{L})^{-1}\hat{A})).
 \end{aligned}$$

## 8. Application of the Liouville Resolvent Method

### 8.1. Evaluation of Diagonal Hamiltonians

Determining the Green function by evaluating matrix elements of the resolvent of the Liouville superoperator can be simple and fairly direct for diagonal Hamiltonian operators. This is especially so if the matrix elements are calculated with respect to an orthonormal basis set of operators such as  $\hat{\phi}_m$  and  $\hat{\phi}_n$ . An outline of the calculations for a simple example follows:

Get the moment expansion of the generalized resolvent:

$$(\omega^k \hat{I} - \hat{L}^k)^{-1} = \frac{1}{\omega^k} \sum_{j=0}^{\infty} \left[ \frac{\hat{L}^k}{\omega^k} \right]^j,$$

$$\begin{aligned} \therefore (\omega^k \hat{I} - \hat{L}^k)^{-1} \hat{\phi}_n &= \frac{1}{\omega^k} \sum_{j=0}^{\infty} \left[ \frac{\hat{L}}{\omega} \right]^{jk} \hat{\phi}_n \\ &= \frac{1}{\omega^k} \sum_{j=0}^{\infty} \frac{\hat{L}^{jk}}{\omega^{jk}} \hat{\phi}_n. \end{aligned}$$

For diagonal  $\hat{H}$  get:

$$\hat{H}_0 \psi_i = E_i \psi_i,$$

$$E_n = E_{i+1} - E_i,$$

$$\hat{L}_0 \hat{\phi}_n = E_n \hat{\phi}_n,$$

$$\hat{L}_0^j \hat{\phi}_n = E_n^j \hat{\phi}_n,$$

$$(\omega \hat{I}^k - \hat{L}^k)^{-1} \hat{\phi}_n = \frac{1}{\omega^k} \sum_{j=0}^{\infty} \left[ \frac{E_n^k}{\omega^k} \right]^j \hat{\phi}_n,$$

$$(\omega \hat{I}^k - \hat{L}^k)^{-1} \hat{\phi}_n = \frac{1}{\omega^k - E_n^k} \hat{\phi}_n.$$

Matrix elements of the resolvent are calculated from inner products by

$$\begin{aligned} & ((\hat{\phi}_m, (\omega \hat{I}^k - \hat{L}^k)^{-1} \hat{\phi}_n)) \\ &= ((\hat{\phi}_m, \frac{1}{(\omega^k - E_n^k)} \hat{\phi}_n)) \\ &= \frac{((\hat{\phi}_m, \hat{\phi}_n))}{(\omega^k - E_n^k)}. \end{aligned}$$

For an orthonormal basis set  $\hat{\phi}$  get:

$$((\hat{\phi}_n, (\omega \hat{I}^k - \hat{L}^k)^{-1} \hat{\phi}_n)) = \frac{\delta_{mn}}{(\omega^k - E_n^k)}.$$

A specific example of a diagonal Hamiltonian operator is

$$\hat{H}_0 = \sum_k \hat{\epsilon}_k \hat{c}_k^\dagger c_k.$$

In order to simplify notation, one-dimensional indices  $k$  and  $q$  will be used instead of the three-dimensional vector indices  $\vec{k}$  and  $\vec{q}$  that would be appropriate for a realistic Hamiltonian, but this will not be of significance in the calculations.

The unit basis vectors are fermion creation operators and fermion stepping operators. Inner products of basis vectors are of the following form:

$$\begin{aligned} ((\hat{\phi}_m, \hat{\phi}_n)) &= ((\hat{c}_q, \hat{c}_k)) \\ &= \langle \{\hat{c}_k, \hat{c}_q^+\} \rangle \\ &= \delta_{kq}. \end{aligned}$$

The Liouville superoperator operates on a basis vector to give

$$\begin{aligned} \hat{L}_0 \hat{\phi}_n &= \hat{L}_0 \hat{c}_k \\ &= [\hat{c}_k, \hat{H}_0] \\ &= \hat{c}_k \hat{H}_0 - \hat{H}_0 \hat{c}_k \\ &= \epsilon_k \sum_k (\hat{c}_k \hat{c}_k^+ \hat{c}_k - \hat{c}_k^+ \hat{c}_k \hat{c}_k). \end{aligned}$$

The product of two fermion annihilation operators is null:

$$\hat{c}_k \hat{c}_q + \hat{c}_q \hat{c}_k = 0 \Rightarrow \hat{c}_k \hat{c}_k = -\hat{c}_k \hat{c}_k \Rightarrow \hat{c}_k \hat{c}_k = 0.$$

The fermion anticommutation relation can simplify the term

$$\hat{c}_k \hat{c}_k^+ \hat{c}_k = (1 - \hat{c}_k^+ \hat{c}_k) \hat{c}_k = \hat{c}_k.$$

The Liouville superoperator for the diagonal Hamiltonian, acting on a basis vector, yields an eigenvalue

equation

$$\hat{L}_0 \hat{c}_k = \epsilon_k \hat{c}_k.$$

Matrix elements of the resolvent are

$$((\hat{\phi}_m, (\omega \hat{I} - \hat{L}_0)^{-1} \hat{\phi}_n)) = \frac{((\hat{\phi}_m, \hat{\phi}_n))}{\omega - E_n},$$

$$\begin{aligned} ((\hat{c}_q, (\omega \hat{I} - \hat{L}_0)^{-1} \hat{c}_k)) &= \frac{((\hat{c}_m, \hat{c}_k))}{\omega - E_k} \\ &= \frac{\delta_{mn}}{\omega - \epsilon_k}. \end{aligned}$$

If the matrix elements are calculated with respect to operators  $\hat{A}$  and  $\hat{B}$  that are not part of an orthonormal basis set, the calculations are only slightly more complicated:

$$\begin{aligned} &(\hat{A}, (\omega \hat{I} - \hat{L})^{-1} \hat{B}) \\ &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{((\hat{A}, \hat{\phi}_m))}{((\hat{\phi}_m, \hat{\phi}_m))} ((\hat{\phi}_m, (\omega \hat{I} - \hat{L})^{-1} \hat{\phi}_n)) \\ &\quad \times \frac{((\hat{\phi}_n, \hat{B}))}{((\hat{\phi}_n, \hat{\phi}_n))} \\ &= \sum_{m=0}^{\infty} \sum_{n=0}^{\infty} \frac{((\hat{A}, \hat{\phi}_m)) ((\hat{\phi}_m, \hat{\phi}_n)) \delta_{mn} ((\hat{\phi}_n, \hat{B}))}{((\hat{\phi}_m, \hat{\phi}_m)) (\omega - E_n) ((\hat{\phi}_n, \hat{\phi}_n))} \\ &= \sum_{n=0}^{\infty} \frac{((\hat{A}, \hat{\phi}_n)) ((\hat{\phi}_n, \hat{B}))}{(\omega - E_n) ((\hat{\phi}_n, \hat{\phi}_n))}. \end{aligned}$$

An orthonormal basis set can be constructed from one

that is not. The usual technique is the Schmidt orthogonalization procedure.

It is possible to calculate the density-density correlation function for the same diagonal Hamiltonian operator

$$\hat{H} = \sum_k \epsilon_k \hat{c}_k^\dagger \hat{c}_k$$

but using for basis operators the densities

$$\hat{\rho}_{p,q} = \hat{c}_p^\dagger \hat{c}_{p+q}$$

The calculations give

$$\begin{aligned} \hat{L}_{\hat{\rho}_{p,q}} &= [\hat{\rho}_{p,q}, \hat{H}] \\ &= (\epsilon_{p+q} - \epsilon_p) \hat{c}_p^\dagger \hat{c}_{p+q}, \\ &((\hat{c}_{p'}^\dagger \hat{c}_{p'+q}, \hat{c}_p^\dagger \hat{c}_{p+q}))_b \\ &= \langle [(\hat{c}_p^\dagger \hat{c}_{p+q}, \hat{H}), \hat{c}_{p'+q}^\dagger \hat{c}_{p'}] \rangle \\ &= \langle [(\epsilon_{p+q} - \epsilon_p) \hat{c}_p^\dagger \hat{c}_{p+q}, \hat{c}_{p'+q}^\dagger \hat{c}_{p'}] \rangle. \end{aligned}$$

Factors in the first term in the commutator on the right-hand side of the equation can be commuted as follows:

$$\begin{aligned} &\hat{c}_p^\dagger (\delta_{pp'} - \hat{c}_{p'+q}^\dagger \hat{c}_{p+q}) \hat{c}_{p'} \\ &= \delta_{pp'} (\hat{c}_p^\dagger \hat{c}_{p'} - \hat{c}_{p'+q}^\dagger \hat{c}_{p+q}) + \hat{c}_{p'+q}^\dagger \hat{c}_{p'} \hat{c}_p^\dagger \hat{c}_{p+q}. \end{aligned}$$

The substitution of this back into the equation produces a "cancellation" of two terms and gives

$$\begin{aligned}
& ((\hat{c}_p^+, \hat{c}_{p+q}, \hat{c}_p^+ \hat{c}_{p+q}))_b \\
& = (\epsilon_{p+q} - \epsilon_p) \delta_{p,p'} \langle (\hat{c}_p^+ \hat{c}_{p'} - \hat{c}_{p'+q}^+ \hat{c}_{p+q}) \rangle.
\end{aligned}$$

The density-density correlation function is

$$A(q, \omega) = \sum_{p,p'} ((\hat{c}_p^+, \hat{c}_{p'+q}, (\omega^2 - L^2)^{-1} \hat{c}_p^+ \hat{c}_{p+q}))_b.$$

The equation for matrix elements of a resolvent gives

$$\begin{aligned}
A(q, \omega) &= \sum_{p,p'} \frac{((\hat{c}_p^+, \hat{c}_{p'+q}, \hat{c}_p^+ \hat{c}_{p+q}))_b}{\omega^2 - (\epsilon_{p+q} - \epsilon_p)^2} \\
&= \sum_p (\epsilon_{p+q} - \epsilon_p) \frac{(N_p - N_{p+q})}{\omega^2 - (\epsilon_{p+q} - \epsilon_p)^2}.
\end{aligned}$$

The density-density correlation function is an example of a spectral function. Spectral functions are discussed in the following section.

## 8.2. Spectral Function

The retarded Green function has been discussed in some detail. Use is sometimes made of other Green functions, including the advanced Green function. The retarded and advanced Green functions for two operators  $\hat{A}$  and  $\hat{B}$  are defined by the following pair of expressions (Rickayzen 1980):

$$G_R(t, t') = -\frac{i}{\hbar} \langle [\hat{A}(t), \hat{B}(t')]_{\eta} \rangle \theta(t - t'),$$

$$G_A(t, t') = + \frac{1}{\hbar} \langle [\hat{A}(t), \hat{B}(t')]_{\eta} \rangle e(t' - t).$$

As has been mentioned,  $\hbar$  is conventionally unitized.

Then the respective Fourier transforms are the following:

$$\begin{aligned} G_R(\omega) &= \lim_{\delta \rightarrow 0^+} G_R(\omega + i\delta) \\ &= \lim_{\delta \rightarrow 0^+} \int_{-\infty}^{\infty} d(t - t') \exp[i(\omega + i\delta)(t - t')] \\ &\quad \times G_R(t, t'), \end{aligned}$$

$$\begin{aligned} G_A(\omega) &= \lim_{\delta \rightarrow 0^+} G_A(\omega - i\delta) \\ &= \lim_{\delta \rightarrow 0^+} \int_{-\infty}^{\infty} d(t - t') \exp[i(\omega - i\delta)(t - t')] \\ &\quad \times G_A(t, t'). \end{aligned}$$

The expression  $G_R(\omega + i\delta)$  is analytic in the upper half of the complex  $z$  plane, while  $G_A(\omega - i\delta)$  is analytic in the lower half of the complex  $z$  plane. By defining a function  $A(x)$  called the spectral function, it is possible to write a single function

$$G(z) = \frac{1}{2\pi} \int_{-\infty}^{\infty} \frac{dx A(x)}{(z - x)}$$

that is analytic and equal to  $G_R(z)$  in the upper-half  $z$  plane and analytic and equal to  $G_A(z)$  in the lower-half  $z$  plane. In general,  $G(z)$  need not be analytic everywhere. It may have a branch cut in the real axis, given by

$$\begin{aligned}
G_R(\omega) - G_A(\omega) &= \lim_{\delta \rightarrow 0} G_R(\omega + i\delta) - \lim_{\delta \rightarrow 0} G_A(\omega - i\delta) \\
&= \lim_{\delta \rightarrow 0} G(\omega + i\delta) - \lim_{\delta \rightarrow 0} G(\omega - i\delta) \\
&= \lim_{\delta \rightarrow 0} [G(\omega + i\delta) - G(\omega - i\delta)] \\
&= \frac{1}{2\pi} \lim_{\delta \rightarrow 0} \int_{-\infty}^{\infty} dx A(x) \\
&\quad \times \left[ \frac{1}{\omega + i\delta - x} - \frac{1}{\omega - i\delta - x} \right] \\
&= -\frac{2\pi i}{2\pi} \int_{-\infty}^{\infty} dx A(x) \delta(x - \omega) \\
&= -iA(\omega).
\end{aligned}$$

The spectral function is

$$\begin{aligned}
A(\omega) &= i \lim_{\delta \rightarrow 0} [G(\omega + i\delta) - G(\omega - i\delta)] \\
&= i \lim_{\delta \rightarrow 0} [(\hat{B}, (\omega + i\delta)\hat{I} - \hat{L})\hat{A} \\
&\quad - ((\hat{B}, (\omega - i\delta)\hat{I} - \hat{L})\hat{A})] \\
&\equiv A[(\hat{B}, (\omega\hat{I} - \hat{L})^{-1}\hat{A})].
\end{aligned}$$

In this notation the brackets contain the argument of and emphasize the dependence of the spectral function of various matrix elements of the resolvent.

A simple example may help to illustrate this relation of the Green function to the spectral function (Kadanoff and Baym 1962). The Green function for a free particle in one

dimension is

$$G(p, z) = \frac{1}{z - p^2/2m}.$$

Using one representation for the delta function (not to be confused here with the variable  $\delta$ ), the spectral function is found to be

$$A(p, \omega) = 2\pi \delta(\omega - p^2/2m).$$

The evaluation of some Green functions can give rise to temperature-dependent matrix elements  $((\hat{A}, \hat{L}\hat{B}))$  involving thermal averages of the form  $\langle \hat{A}^+ \hat{B} \rangle$ . These thermal averages can be expressed in terms of the spectral function and the appropriate version of the function

$$f(\omega) = \frac{1}{1 + \eta \exp[\beta(\omega - N\mu)]},$$

where  $N$  is the change in the number of particles. The function is the Bose function for

$$\eta = -1$$

or the Fermi function for

$$\eta = +1.$$

The thermal averages are calculated as follows:

$$\begin{aligned} \langle \hat{A}^+ \hat{B} \rangle &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) A(\omega) \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) A[(\hat{B}, (\omega \hat{I} - \hat{L})^{-1} \hat{A})] \end{aligned}$$

$$= \sum_{n=0}^{\infty} f(E_n) \frac{((\hat{B}, \hat{\phi}_n))((\hat{\phi}_n, \hat{A}))}{((\hat{\phi}_n, \hat{\phi}_n))},$$

if  $\hat{\phi}_n$  is an eigenvector of  $\hat{L}$  with eigenvalue  $E_n$ .

For some physical models, there are no thermal averages on the right-hand side of this equation, and the thermodynamics is completely closed. For other models, thermal averages do appear on the right, so the thermodynamics can then be found only by the solution of coupled linear inhomogeneous equations, which must be solved for individual correlation functions in terms of the Bose or Fermi function.

An interesting example of thermal averages of the form  $\langle \hat{A}^+ \hat{B} \rangle$  is

$$\begin{aligned} \langle \hat{\phi}_n^+ \hat{\phi}_n \rangle &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) A(\omega) \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) A[ ((\hat{\phi}_n, (\omega \hat{I} - \hat{L})^{-1} \hat{\phi}_n)) ] \\ &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) ((\hat{\phi}_n, \hat{\phi}_n)) \delta(\omega - E_n) \end{aligned}$$

if  $\hat{\phi}_n$  is an eigenvector of  $\hat{L}$ . So

$$\begin{aligned} \langle \hat{\phi}_n^+ \hat{\phi}_n \rangle &= ((\hat{\phi}_n, \hat{\phi}_n)) f(E_n) \\ &= \langle (\hat{\phi}_n, \hat{\phi}_n^+) \rangle f(E_n) \end{aligned}$$

$$\begin{aligned}
&= (\langle \hat{\phi}_n \hat{\phi}_n^+ \rangle + \langle \hat{\phi}_n^+ \hat{\phi}_n \rangle) f(E_n), \\
\therefore \langle \hat{\phi}_n^+ \hat{\phi}_n \rangle [1 - f(E_n)] &= \langle \hat{\phi}_n \hat{\phi}_n^+ \rangle f(E_n), \\
\langle \hat{\phi}_n^+ \hat{\phi}_n \rangle &= \frac{f(E_n)}{1 - f(E_n)} \langle \hat{\phi}_n \hat{\phi}_n^+ \rangle.
\end{aligned}$$

By considering all such ratios for the complete set of eigenvectors of  $\hat{L}$  it can be seen that this set of equations is equivalent to knowledge of the partition function.

## 9. Approximate Solutions

### 9.1. Discussion

The selection of Judd operators is usually an important step in the application of the Liouville resolvent method. The selection of appropriate Judd operators is as much an art as a science. In some simple cases, a serendipitous choice may result in immediate diagonalization of the Hamiltonian operator. In other cases, the best choice that can be found is one that most nearly diagonalizes the Hamiltonian operator.

In the Judd procedure, a stepping operator

$$\hat{c} = \sum_i b_i \hat{\Psi}_i$$

is expressed in terms of eigenstates  $\hat{\Psi}_i$  of the Liouville superoperator, as indicated by the equation

$$\hat{L}\hat{\Psi}_i = \lambda_i \hat{\Psi}_i.$$

The eigenstates  $\hat{\Psi}_i$  are expressed as linear combinations of Judd operators  $\hat{\phi}$  that step between Fock-space states with  $N+1$  and  $N$  particles. The Judd operators are thus stepping operators between many-particle states. These operators manifest the properties of many-particle systems.

Solving the eigenvalue problem for  $\hat{L}$  simultaneously diagonalizes the resolvent matrix for  $\hat{L}$ . The

diagonalization is made easier by the symmetry properties of the Hamiltonian operator and by the Lie group structure of the Judd operators.

The Liouville resolvent method amounts to solving the eigenvalue equation of  $\hat{L}$  and expressing the single-particle Green function as

$$G(\omega) = \sum_i \frac{|b_i|^2}{\omega - \lambda_i} ((\hat{\Psi}_i, \hat{\Psi}_i))$$

with

$$((\hat{\Psi}_i, \hat{\Psi}_j)) = 0, \quad i \neq j.$$

The definition of the scalar product in superspace leads to the expression of the Green function as a sum of thermal averages of various correlation functions. Coupled equations of a general form similar to

$$\langle \hat{\Psi}_i^\dagger \hat{\Psi}_i \rangle = f(\lambda_i) ((\hat{\Psi}_i, \hat{\Psi}_i))$$

must be solved for individual correlation functions in terms of Bose or Fermi functions  $f(\lambda_i)$ . (A reference is Mancini, J. D. 1982. Judd operator methods in superspace. Diss. Va. Tech.)

The overall procedure may still seem straightforward even if  $\hat{L}$  must be diagonalized, but the process of diagonalization, except in those simple cases where it is readily accomplished, necessitates the introduction of

further complication, and in practice usually requires approximate solutions.

## 9.2. Truncation Approximations

The material in this section closely paraphrases the literature (Masson 1970; Bowen et al. 1984).

For complex

$$z = \omega + i\delta$$

farther than some small distance  $\delta$  from the real axis, and for an  $H$ , the domain of which is an infinite-dimensional Hilbert space, there is a matrix dimension  $N(\delta)$  such that matrix elements of resolvents of  $N \times N$  matrices  $\underline{H}_N$ , where  $N > N(\delta)$ , give approximations to the corresponding exact matrix elements of the resolvent that are as close as desired for large enough  $N$ . This is a consequence of Masson's theorem, which guarantees the following convergence of matrix elements:

$$\begin{aligned} R_{nm}(\omega + i\delta) &= \langle \Psi_n | [(\omega + i\delta)\hat{I} - \hat{H}]^{-1} | \Psi_m \rangle \\ &= \lim_{N \rightarrow \infty} \langle \Psi_n | [(\omega + i\delta)\underline{I}_N - \underline{H}_N]^{-1} | \Psi_m \rangle. \end{aligned}$$

The  $\delta$  is a measure of the resolution or resolving power of the approximation. For a chosen  $\delta$ , sequences of approximants with increasing  $N$  can be built to approach the exact solution.

The determination of a matrix element of

$$((\hat{A}, (z\hat{I} - \hat{L})^{-1}\hat{B}))$$

involves choosing a resolving power  $\delta$  and computing  $N \times N$  secular matrices

$$((\hat{\phi}_n, (z\hat{I} - \hat{L})\hat{\phi}_m))$$

with respect to an orthonormal basis set of  $N$  second-quantized operators  $\hat{\phi}_n$  that are chosen to be a basis for expanding  $\hat{A}$  and  $\hat{B}$  approximately in the operator Hilbert space and are also chosen to make the secular matrix of  $\hat{L}$  as nearly diagonal as possible. For large enough  $N$ , the resolvents of these finite  $N \times N$  truncations of the secular matrix of  $\hat{L}$  with respect to a basis of many-particle operators are accurate approximations to corresponding matrix elements of the exact resolvent at  $z = \omega + i\delta$ . The physics and the art of a particular approximation reside in the selection of the orthonormal basis set  $\hat{\phi}_n$  of second-quantized operators.

Quantities of interest such as

$$\langle \hat{A}^+ \hat{B} \rangle = \int \frac{d\omega}{2\pi} f(\omega) A[(\hat{B}, (\omega\hat{I} - \hat{L})^{-1}\hat{A})]$$

are approximated in principle by using a nonzero value of  $\delta$  and an  $N \times N$  truncation.

### 9.3. Feenberg Formulas

Exact analytic formulas can be written down for the resolvent in terms of diagonal and off-diagonal matrix elements of  $L$  (Feenberg 1948; Dyson 1952; Bowen et al. 1984).

Corresponding to a Hamiltonian operator  $\hat{H}$  there is a Liouville superoperator

$$\hat{L} = \hat{L}_0 + \hat{V}$$

where  $\hat{L}_0$  is diagonal and  $\hat{V}$  has only off-diagonal matrix elements.

For an orthonormal basis set  $|n\rangle$ , diagonal matrix elements are

$$V_{nm} = \langle n | \hat{V} | m \rangle.$$

Using the Kronecker delta, the matrix elements of  $\hat{L}$  are written as

$$L_{nm} = \delta_{nm} E_n + V_{nm}.$$

The diagonal matrix elements of the resolvent of  $\hat{L}$  are (using the subscript index as an abbreviated notation for a state)

$$\begin{aligned} \langle n | [(\omega + i\delta)\hat{I} - \hat{L}]^{-1} | n \rangle \\ = [\omega + i\delta - e_n(\omega + i\delta)]^{-1}. \end{aligned}$$

The off-diagonal matrix elements of the resolvent of  $\hat{L}$

are

$$\begin{aligned} \langle n | (\omega \hat{I} - \hat{L})^{-1} | m \rangle \\ = [\omega - e_n(\omega)]^{-1} T_{nm} [\omega - e_m(n; \omega)]^{-1}. \end{aligned}$$

The reduced self-energy of the  $n$ th state is

$$e_n(\omega) = E_n + \Sigma_n(\omega).$$

The self-energy of the  $n$ th state is

$$\begin{aligned} \Sigma_n(\omega) = \sum_{m \neq n} \frac{|V_{nm}|^2}{\omega - e_m(n; \omega)} \\ + \sum_{\substack{m \neq n \\ m' \neq n, m}} \frac{V_{nm} V_{mm'} V_{m'n}}{[\omega - e_m(n; \omega)][\omega - e_{m'}(n, m; \omega)]} \\ + \dots \end{aligned}$$

The sum-restricted T matrix is

$$\begin{aligned} T_{nn'} = V_{n,n'} + \sum_{m \neq n, n'} \frac{V_{nm} V_{mn'}}{\omega - e_m(n, n'; \omega)} \\ + \sum_{\substack{m \neq n, m' \\ m' \neq n, n', m}} \frac{V_{nm} V_{mm'} V_{m'n'}}{[\omega - e_m(n, n'; \omega)]} \\ \times \frac{1}{[\omega - e_{m'}(n, n', m; \omega)]} \\ + \dots \end{aligned}$$

The reduced self-energies  $e_m(n; \omega)$  and  $e_{m'}(n, m; \omega)$  are like  $e_n(\omega)$  except that any state indices preceding a semicolon cannot be included in a sum.

For any  $N \times N$  truncation of  $\hat{L}$  the expression for the

self-energy  $\Sigma_n(\omega)$  contains only a finite number of terms and the last term in the sum contains  $N$  factors of  $V$ . The expression is equivalent to the formula for the  $mn$  element of an inverse matrix obtained by using the Laplace expansion in terms of signed minors.

The sum-restricted  $T$  matrix is similar to the usual  $T$  matrix defined for the Born series, but the summation restrictions restrict the poles and singularities of the  $T$  matrix and ensure convergence of the approximants.

#### 9.4. Summary of Method

Following is a sequence of steps used in applying the Liouville resolvent method:

$$(1) \quad \hat{H} = f(\hat{A}) \vee \hat{A},$$

$$(2) \quad \hat{L}\hat{A} = [\hat{A}, \hat{H}] \Rightarrow \hat{A}_1,$$

$$(3) \quad \left. \begin{aligned} \hat{\phi}_1 &= \frac{\hat{A}_1}{\|\hat{A}_1\|} \\ \hat{\phi}_2 &= \frac{\hat{A}_2 - ((\hat{\phi}_1, \hat{A}_2))\hat{\phi}_1}{\|\hat{A}_2 - ((\hat{\phi}_1, \hat{A}_2))\hat{\phi}_1\|} \\ &\dots \end{aligned} \right\} \Rightarrow \hat{\phi}_1,$$

$$(4) \quad \hat{T} = \omega\hat{I} - \hat{L},$$

$$T_{ki} = \frac{((\hat{\phi}_k, (\omega\hat{I} - \hat{L})\hat{\phi}_i))}{((\hat{\phi}_k, \hat{\phi}_k))}$$

$$= \delta_{ki} \omega \hat{I} - \frac{((\hat{\phi}_k, \hat{L}\hat{\phi}_i))}{((\hat{\phi}_k, \hat{\phi}_k))},$$

$$(5) \quad \delta_{ji} = \sum_k (T^{-1})_{jk} T_{ki} \Rightarrow (T^{-1})_{jk},$$

$$(T^{-1})_{jk} = ((\hat{\phi}_j, (\omega \hat{I} - \hat{L})^{-1} \hat{\phi}_k))$$

$$= G,$$

$$(6) \quad A_\delta(\omega) = i((\hat{\phi}_j, [(\omega + i\delta)\hat{I} - \hat{L}]^{-1} \hat{\phi}_k)) \\ - ((\hat{\phi}_j, [(\omega - i\delta)\hat{I} - \hat{L}]^{-1} \hat{\phi}_k)),$$

$$(7) \quad \langle \phi_k^\dagger \phi_j \rangle = \lim_{\delta \rightarrow 0} \int \frac{d\omega}{2\pi} f(\omega) A_\delta(\omega),$$

(8) Iterate with

$$\hat{L}\hat{A}_1 \Rightarrow \hat{A}_1, \hat{A}_j,$$

i.e.

$$\hat{L}^n \hat{A} \Rightarrow \hat{A}_1, \hat{A}_j, \dots$$

It should be noted that the division by inner products in step (4), which would be done to ensure normalization, is redundant if the normalization of the  $\hat{\phi}_k$  has been accomplished by the Gram-Schmidt orthonormalization procedure of step (3).

Following is a procedure for finding  $(T^{-1})_{jk}$ :

$$\hat{T} = \omega \hat{I} - \hat{L},$$

$$\hat{\mathbb{T}}\hat{\phi}_i = \sum_k T_{ki} \hat{\phi}_k,$$

$$T_{ki} = \frac{((\hat{\phi}_k, (\omega\hat{\mathbb{I}} - \hat{\mathbb{L}})\hat{\phi}_i))}{((\hat{\phi}_k, \hat{\phi}_k))}$$

$$= \delta_{ki}\omega - \frac{((\hat{\phi}_k, \hat{\mathbb{L}}\hat{\phi}_k))}{((\hat{\phi}_k, \hat{\phi}_k))},$$

$$\hat{\mathbb{T}}^{-1} = (\omega\hat{\mathbb{I}} - \hat{\mathbb{L}})^{-1},$$

$$\hat{\mathbb{T}}^{-1}\hat{\phi}_k = \sum_j (T^{-1})_{jk} \hat{\phi}_j,$$

$$\phi_i = \sum_{k,j} (T^{-1})_{jk} T_{ki} \hat{\phi}_j.$$

Then  $(T^{-1})_{jk}$  is found by solving the set of simultaneous equations:

$$\delta_{ji} = \sum_k (T^{-1})_{jk} T_{ki}.$$

### 9.5. Solutions to First Order

The solution for  $\underline{\mathbb{T}}^{-1}$  to first order in the stepping operators uses

$$j = 1, m;$$

$$k = u, v;$$

$$i = 1, m;$$

$$T_{ki} = \begin{bmatrix} T_{ul} & T_{um} \\ T_{vl} & T_{vm} \end{bmatrix}.$$

The matrix elements are these:

$$(T^{-1})_{lv} = \frac{1}{T_{vl} - T_{vm}T_{ul}/T_{um}},$$

$$(T^{-1})_{lu} = \frac{-(T^{-1})_{lv}T_{vm}}{T_{um}},$$

$$(T^{-1})_{mv} = \frac{1}{T_{vm} - T_{vl}T_{um}/T_{ul}},$$

$$(T^{-1})_{mu} = \frac{-(T^{-1})_{mv}T_{vl}}{T_{ul}}.$$

It is sometimes convenient to use the substitution

$$R_{ki} \equiv \omega - T_{ki}.$$

For the special case  $k = i = 1$  it is possible to write

$$\begin{aligned} (T^{-1})_{11} &= \frac{1}{T_{11} - T_{12}T_{21}/T_{22}} \\ &= \omega - R_{11} - \frac{T_{12}T_{21}}{\omega - R_{22}} \\ &= \frac{\omega - R_{22}}{\omega^2 - (R_{11} + R_{22})\omega + (R_{11}R_{22} - T_{12}T_{21})}. \end{aligned}$$

If

$$E_A = R_{22},$$

$$E_{P,M} = \frac{R_{11} + R_{22}}{2} \pm \sqrt{\left[\frac{R_{11} - R_{22}}{2}\right]^2 + T_{12}T_{21}}$$

then

$$(T^{-1})_{11} = \frac{\omega - E_A}{(\omega - E_P)(\omega - E_M)}.$$

The corresponding spectral function is

$$\begin{aligned} A[(T)^{-1}_{11}] &= i \left[ \frac{\omega + i\delta - E_A}{E_P - E_M} \right] \\ &\quad \times \left[ \frac{1}{\omega + i\delta - E_P} - \frac{1}{\omega + i\delta - E_M} \right] \\ &\quad - i \left[ \frac{\omega - i\delta - E_A}{E_P - E_M} \right] \\ &\quad \times \left[ \frac{1}{\omega - i\delta - E_P} - \frac{1}{\omega - i\delta - E_M} \right] \\ &= \frac{(E_P - E_A)2\delta}{(E_P - E_M)[(\omega - E_P)^2 + \delta^2]} \\ &\quad - \frac{(E_M - E_A)2\delta}{(E_P - E_M)[(\omega - E_A)^2 + \delta^2]} \\ &= \frac{(E_P - E_A)}{(E_P - E_M)} 2\pi\delta(\omega - E_P) \\ &\quad - \frac{(E_P - E_A)}{(E_P - E_M)} 2\pi\delta(\omega - E_M) \end{aligned}$$

in terms of Dirac delta functions.

From the preceding it is possible to calculate expectation values of the form

$$\langle \hat{\phi}_1^\dagger \hat{\phi}_1 \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} f(\omega) A[(T^{-1})_{11}]$$

$$\begin{aligned}
&= \frac{(E_P - E_A)}{(E_P - E_M)} \int_{-\infty}^{\infty} d\omega f(\omega) \delta(\omega - E_P) \\
&\quad - \frac{(E_M - E_A)}{(E_P - E_M)} \int_{-\infty}^{\infty} d\omega f(\omega) \delta(\omega - E_M) \\
&= \frac{(E_P - E_A)}{(E_P - E_M)} f(E_P) - \frac{(E_M - E_A)}{(E_P - E_M)} f(E_M).
\end{aligned}$$

### 9.6. Partial Solution to Second Order

The solution for  $\underline{T}^{-1}$  to second order in the stepping operators uses

$$j = l, m, n;$$

$$k = u, v, w;$$

$$i = l, m, n.$$

The matrix elements of the first row of  $\underline{T}^{-1}$  are these:

$$(T^{-1})_{lv} = (T^{-1})_{lu} \frac{(-T_{um} + T_{un}T_{wm}/T_{wn})}{(T_{vm} - T_{vn}T_{wm}/T_{wn})},$$

$$(T^{-1})_{lw} = (T^{-1})_{lu} \frac{(-T_{un} + T_{um}T_{vn}/T_{vm})}{(T_{wn} - T_{wm}T_{vn}/T_{vm})},$$

$$\begin{aligned}
(T^{-1})_{lu} = & \left[ T_{ul} + \frac{T_{um}(T_{wl}T_{vn} - T_{vl}T_{wn})}{T_{vm}T_{wn} - T_{vn}T_{wm}} \right. \\
& \left. + \frac{T_{um}(T_{vl}T_{wm} - T_{wl}T_{vm})}{T_{vm}T_{wn} - T_{vn}T_{wm}} \right]^{-1}.
\end{aligned}$$

As could be guessed from the solutions to first order, the solutions for  $[(T^{-1})_{mu}]$ ,  $[(T^{-1})_{mv}]$ , and  $[(T^{-1})_{mw}]$  can be found from the preceding by replacing each  $l$  by  $m$  and vice versa and the solutions for  $[(T^{-1})_{nu}]$ ,  $[(T^{-1})_{nv}]$ , and

$[(T^{-1})_{nw}]$  can be found by replacing each 1 by n and vice versa.

The spectral function and the expectation values are not obtained as simply for second order as they are for first order.

### 9.7. Relation of Zubarev and Liouville Methods

Consider the identity

$$(\omega \hat{I} - \hat{L})^{-1} (\omega \hat{I} - \hat{L}) = \hat{I}. \quad (9.1)$$

It is possible to commute quantities so Eq. (9.1) can be rewritten in the form

$$\omega (\omega \hat{I} - \hat{L})^{-1} = \hat{I} + (\omega \hat{I} - \hat{L})^{-1} \hat{L}. \quad (9.2)$$

It is then possible to calculate Green functions from Eq. (9.2) to get

$$\begin{aligned} \omega \langle (\hat{B}, (\omega \hat{I} - \hat{L})^{-1} \hat{A}) \rangle &= \langle (\hat{B}, \hat{A}) \rangle \\ &+ \langle (\hat{B}, (\omega \hat{I} - \hat{L})^{-1} \hat{L} \hat{A}) \rangle. \end{aligned} \quad (9.3)$$

In Zubarev notation Eq. (9.3) can be written in the form

$$\omega \langle \langle \hat{A}; \hat{B}^+ \rangle \rangle_{\omega} = \langle \langle \hat{A}, \hat{B}^+ \rangle \rangle + \langle \langle \hat{L} \hat{A}, \hat{B}^+ \rangle \rangle_{\omega}. \quad (9.4)$$

The second term on the right-hand side of Eq. (9.3) can be expressed in terms of an orthonormal basis set  $\hat{\phi}_n$ , with the term  $\hat{\phi}_1$  written as  $\hat{A}$ , by the relation

$$\begin{aligned}
((\hat{B}, (\omega\hat{I} - \hat{L})^{-1}\hat{L}\hat{A})) &= \sum_n ((\hat{B}, (\omega\hat{I} - \hat{L})^{-1}\hat{\phi}_n)) \\
&\times ((\hat{\phi}_n, \hat{L}\hat{\phi}_1)). \quad (9.5)
\end{aligned}$$

Substitution of Eq. (9.5) into Eq. (9.3) leads to the equation

$$\begin{aligned}
\sum_n ((\hat{B}, (\omega\hat{I} - \hat{L})^{-1}\hat{\phi}_n))(\omega\delta_{n1} - ((\hat{\phi}_n, \hat{L}\hat{\phi}_1))) \\
= ((\hat{B}, \hat{\phi}_1)). \quad (9.6)
\end{aligned}$$

Eq. (9.6) is of the form

$$\sum_n (T^{-1})_{Bn} T_{n1} = ((\hat{B}, \hat{\phi}_1)). \quad (9.7)$$

This relation expressed by Eq. (9.7) is equivalent to a unitary transformation. Relations of this form are used in the implementation of the Liouville resolvent method.

The relation expressed by Eq. (9.4), on the other hand, is the prime ingredient of the Zubarev method of decoupling factors. The connection between Eq. (9.4) and Eq. (9.7) links the Zubarev method to the Liouville method. If there were a systematic way of making an appropriate choice of decoupling factors in the Zubarev method, this method might be made essentially equivalent to the Liouville method.

## 10. Truncated Solution for Lee Model

### 10.1. Specification of Basis States

A particular variant of the Lee Hamiltonian operator is

$$\hat{H} = \epsilon_0 (\hat{b}^\dagger \hat{b} - \hat{c}^\dagger \hat{c}) + \lambda_0 \omega_0 (\hat{b}^\dagger \hat{c} \hat{a} + \hat{c}^\dagger \hat{b} \hat{a}^\dagger) + \omega_0 \hat{a}^\dagger \hat{a}.$$

The basis states can be labelled  $\hat{\phi}_{ni}$ ; with  $n$  being respectively set equal to  $a$  for bosons,  $b$  for one kind of fermion, and  $c$  for another kind of fermion; and with  $i$  being a positive integer. There are six basis states for the truncation in which  $i$  is limited to 1 and 2:

$$\hat{\phi}_{a1} = \hat{a}, \quad \text{Bose;}$$

$$\left. \begin{aligned} \hat{\phi}_{b1} &= \hat{b} \\ \hat{\phi}_{c1} &= \hat{c} \end{aligned} \right\}, \quad \text{Fermi;}$$

$$\hat{\phi}_{a2} = \hat{c}^\dagger \hat{b}, \quad \text{Bose;}$$

$$\left. \begin{aligned} \hat{\phi}_{b2} &= \hat{a} \hat{c} \\ \hat{\phi}_{c2} &= \hat{a}^\dagger \hat{b} \end{aligned} \right\}, \quad \text{Fermi.}$$

The basis states are not normalized here.

Normalization will be taken into account by the inner products used in the calculation of the  $T_{nij}$ .

Operation on the basis states with the Liouville superoperator gives the following :

$$\hat{L}\hat{\phi}_{a1} = \omega_0\hat{\phi}_{a1} + \lambda_0\omega_0\hat{\phi}_{a2},$$

$$\hat{L}\hat{\phi}_{b1} = \epsilon_0\hat{\phi}_{b1} + \lambda_0\omega_0\hat{\phi}_{b2},$$

$$\hat{L}\hat{\phi}_{c1} = -\epsilon_0\hat{\phi}_{c1} + \lambda_0\omega_0\hat{\phi}_{c2};$$

$$\hat{L}\hat{\phi}_{a2} = 2\epsilon_0\hat{\phi}_{a2} + \lambda_0\omega_0(N_c - N_b)\hat{\phi}_{a1},$$

$$\hat{L}\hat{\phi}_{b2} = (\omega_0 - \epsilon_0)\hat{\phi}_{b2} + \lambda_0\omega_0(1 + N_a - N_b)\hat{\phi}_{b1},$$

$$\hat{L}\hat{\phi}_{c2} = (\epsilon_0 - \omega_0)\hat{\phi}_{c2} + \lambda_0\omega_0(N_a + N_b)\hat{\phi}_{c1}.$$

## 10.2. Calculation of Inner Products

Inner products are the following:

$$((\hat{\phi}_{a1}, \hat{L}\hat{\phi}_{a1})) = \langle [\hat{L}\hat{a}, \hat{a}^+] \rangle = \omega_0,$$

$$((\hat{\phi}_{a1}, \hat{L}\hat{\phi}_{a2})) = \langle [\hat{L}\hat{c}^+\hat{b}, \hat{a}^+] \rangle = \lambda_0\omega_0(N_c - N_b),$$

$$((\hat{\phi}_{a2}, \hat{L}\hat{\phi}_{a1})) = \langle [\hat{L}\hat{a}, \hat{b}^+\hat{c}] \rangle = \lambda_0\omega_0(N_c - N_b),$$

$$((\hat{\phi}_{a2}, \hat{L}\hat{\phi}_{a2})) = \langle [\hat{L}\hat{c}^+\hat{b}, \hat{b}^+\hat{c}] \rangle$$

$$= 2\epsilon_0(N_c - N_b) - 2\lambda_0\omega_0\langle \hat{a}\hat{b}^+\hat{c} \rangle;$$

$$((\hat{\phi}_{b1}, \hat{L}\hat{\phi}_{b1})) = \langle \{\hat{L}\hat{b}, \hat{b}^+\} \rangle = \epsilon_0,$$

$$((\hat{\phi}_{b1}, \hat{L}\hat{\phi}_{b2})) = \langle \{\hat{L}\hat{a}\hat{c}, \hat{b}^+\} \rangle = \lambda_0 \omega_0 (1 + N_a - N_c),$$

$$((\hat{\phi}_{b2}, \hat{L}\hat{\phi}_{b1})) = \langle \{\hat{L}\hat{b}, \hat{c}^+\hat{a}^+\} \rangle = \lambda_0 \omega_0 (1 + N_a - N_c),$$

$$\begin{aligned} ((\hat{\phi}_{b2}, \hat{L}\hat{\phi}_{b2})) &= \langle \{\hat{L}\hat{a}\hat{c}, \hat{c}^+\hat{a}^+\} \rangle \\ &= (\omega_0 - \epsilon_0)(1 + N_a - N_c); \end{aligned}$$

$$((\hat{\phi}_{c1}, \hat{L}\hat{\phi}_{c1})) = \langle \{\hat{L}\hat{c}, \hat{c}^+\} \rangle = -\epsilon_0,$$

$$((\hat{\phi}_{c1}, \hat{L}\hat{\phi}_{c2})) = \langle \{\hat{L}\hat{a}^+\hat{b}, \hat{c}^+\} \rangle = \lambda_0 \omega_0 (N_a + N_b),$$

$$((\hat{\phi}_{c2}, \hat{L}\hat{\phi}_{c1})) = \langle \{\hat{L}\hat{c}, \hat{b}^+\hat{a}^+\} \rangle = \lambda_0 \omega_0 (N_a - N_b),$$

$$\begin{aligned} ((\hat{\phi}_{c2}, \hat{L}\hat{\phi}_{c2})) &= \langle \{\hat{L}\hat{a}^+\hat{b}, \hat{b}^+\hat{a}^+\} \rangle \\ &= (\epsilon_0 - \omega_0)(N_a + N_b). \end{aligned}$$

### 10.3. Calculation of Resolvent Matrix Elements

The inner products are used to calculate the

$$T_{nij} = \delta_{ij} \omega - \frac{((\hat{\phi}_{ni}, \hat{L}\hat{\phi}_{nj}))}{((\hat{\phi}_{ni}, \hat{\phi}_{ni}))} :$$

$$T_{a11} = \omega - \omega_0,$$

$$T_{a12} = \lambda_0 \omega_0 (N_b - N_c),$$

$$T_{a21} = -\lambda_0 \omega_0,$$

$$T_{a22} = \omega - 2\epsilon_0 + \frac{2\lambda_0 \omega_0 \langle \hat{a} \hat{b} \hat{c} \rangle}{N_c - N_b};$$

$$T_{b11} = \omega = \epsilon_0,$$

$$T_{b12} = -\lambda_0 \omega_0 (1 + N_a - N_c),$$

$$T_{b21} = -\lambda_0 \omega_0,$$

$$T_{b22} = \omega - (\omega_0 - \epsilon_0);$$

$$T_{c11} = \omega + \epsilon_0,$$

$$T_{c12} = -\lambda_0 \omega_0 (N_a + N_b),$$

$$T_{c21} = -\lambda_0 \omega_0,$$

$$T_{c22} = \omega + (\omega_0 - \epsilon_0).$$

#### 10.4. Construction of Green Functions

The Green functions, incidentally, are these:

$$(T_n^{-1})_{11} = \frac{1}{T_{n11} - \frac{T_{n12} T_{n21}}{T_{n22}}},$$

$$(T_a^{-1})_{11} = \frac{1}{\omega - \omega_0 - \frac{(\lambda_0 \omega_0)^2 (N_c - N_b)}{\omega - 2\epsilon_0 + \frac{2\lambda_0 \omega_0 \langle \hat{a} \hat{b} \hat{c} \rangle}{N_c - N_b}}},$$

$$(T_b^{-1})_{11} = \frac{1}{\omega - \epsilon_0 - \frac{(\lambda_0 \omega_0)^2 (1 + N_a - N_c)}{\omega - (\omega_0 - \epsilon_0)}},$$

$$(T_c^{-1})_{11} = \frac{1}{\omega + \epsilon_0 - \frac{(\lambda_0 \omega_0)^2 (N_a + N_b)}{\omega + (\omega_0 - \epsilon_0)}}.$$

### 10.5. Calculation of Particle Number

The expectation value of the number operator is calculated from these expressions (ignoring  $\mu$ ):

$$E_A = \omega - T_{n22},$$

$$E_P - E_M = 2 \left[ \left[ \frac{T_{n22} - T_{n11}}{2} \right]^2 + T_{n12} T_{n21} \right]^{1/2},$$

$$E_P - E_A = \left[ \frac{T_{n22} - T_{n11}}{2} \right] + \frac{[E_P - E_M]}{2},$$

$$E_M - E_A = \left[ \frac{T_{n22} - T_{n11}}{2} \right] - \frac{[E_P - E_M]}{2},$$

$$N_n = \left[ \frac{E_P - E_A}{E_P - E_M} \right] \left[ \frac{1}{e^{\beta E_P} + 1} \right] \\ - \left[ \frac{E_M - E_A}{E_P - E_M} \right] \left[ \frac{1}{e^{\beta E_M} + 1} \right].$$

For  $\hat{b}$ :

$$N_b = \frac{1}{2 \left[ 1 + \frac{2(\lambda_0 \omega_0)^2 (1 + N_a - N_c)}{2\epsilon_0 - \omega_0} \right]^{1/2}}$$

$$\times \left[ \frac{1}{e^{\beta E_P} + 1} - \frac{1}{e^{\beta E_M} + 1} \right]$$

$$+ \frac{1}{2} \left[ \frac{1}{e^{\beta E_P} + 1} + \frac{1}{e^{\beta E_M} + 1} \right],$$

$$E_{P,M} = \frac{\omega_0}{2} \pm \left[ \left[ \epsilon_0 - \frac{\omega_0}{2} \right]^2 \right. \\ \left. + (\lambda_0 \omega_0)^2 (1 + N_a - N_c) \right]^{1/2}.$$

For  $\hat{c}$ :

$$N_c = \frac{1}{2 \left[ 1 + \frac{2(\lambda_0 \omega_0)^2 (N_a + N_b)}{\omega_0 - 2\epsilon_0} \right]^{1/2}}$$

$$\times \left[ \frac{1}{e^{\beta E_P} + 1} - \frac{1}{e^{\beta E_M} + 1} \right]$$

$$+ \frac{1}{2} \left[ \frac{1}{e^{\beta E_P} + 1} + \frac{1}{e^{\beta E_M} + 1} \right]$$

$$E_{P,M} = -\frac{\omega_0}{2} \pm \left[ \left[ \frac{\omega_0 - 2\epsilon_0}{2} \right]^2 \right. \\ \left. + (\lambda_0 \omega_0)^2 (N_a + N_b) \right]^{1/2}.$$

For  $\hat{a}$ :

$$N_a = \frac{1}{2 \left[ 1 + \frac{2(\lambda_0 \omega_0)^2 (N_c - N_b)}{\omega_0 - 2\epsilon_0 + \frac{2\lambda_0 \omega_0 \langle \hat{a}\hat{b} + \hat{c} \rangle}{(N_c - N_b)}} \right]^{1/2}}$$

$$\begin{aligned}
& \times \left[ \frac{1}{e^{\beta E_P} - 1} - \frac{1}{e^{\beta E_M} - 1} \right] \\
& + \frac{1}{2} \left[ \frac{1}{e^{\beta E_P} - 1} + \frac{1}{e^{\beta E_M} - 1} \right], \\
E_{P,M} = \epsilon_0 + \frac{\omega_0}{2} + \frac{\lambda_0 \omega_0 \langle \hat{a} \hat{b}^\dagger \hat{c} \rangle}{N_c - N_b} \\
& \pm \left[ -\epsilon_0 + \frac{\omega_0}{2} + \frac{\lambda_0 \omega_0 \langle \hat{a} \hat{b}^\dagger \hat{c} \rangle}{N_c - N_b} \right. \\
& \left. + (\lambda_0 \omega_0)^2 (N_c - N_b) \right]^{1/2}.
\end{aligned}$$

### 10.6. Evaluation of the Binding Energy Term

When  $\lambda_0$  is finite, the equations for the different  $N_n$  are coupled:

$$N_a = N_a(N_b, N_c),$$

$$N_b = N_b(N_a, N_c),$$

$$N_c = N_c(N_a, N_b).$$

Furthermore,  $N_a$  involves the binding energy term  $\langle \hat{a} \hat{b}^\dagger \hat{c} \rangle$ .

How could this be evaluated?

Using

$$\hat{\phi}_{a1} = \hat{a},$$

$$\hat{\phi}_{a2} = \hat{c}^\dagger \hat{b},$$

$$\langle \hat{a}\hat{b}^+\hat{c} \rangle = \langle \hat{\phi}_{a1} \hat{\phi}_{a2}^+ \rangle,$$

unfortunately leads to a complicated equation in  $\langle \hat{a}\hat{b}^+\hat{c} \rangle$  because  $\langle \hat{a}\hat{b}^+\hat{c} \rangle$  appears in  $(T_a^{-1})_{21}$ . It may be more convenient to work with an alternative expression for  $\langle \hat{a}\hat{b}^+\hat{c} \rangle$ .

From commutation properties of  $\hat{a}$ ,  $\hat{b}$  and  $\hat{c}$  it is possible to write

$$\langle \hat{a} | \hat{b}^+\hat{c} \rangle = -\langle \hat{c}\hat{a} | \hat{b}^+ \rangle = -\langle \hat{c} | \hat{b}^+\hat{a} \rangle.$$

The first of this triad has just been considered. The triad can be expressed as

$$\langle \hat{a} | \hat{b}^+\hat{c} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{e^{\beta\omega} - 1} A[(T_a^{-1})_{21}],$$

$$(T_a^{-1})_{21} = -\frac{T_{a21}}{T_{a22}} (T_a^{-1})_{11};$$

$$\langle \hat{c}\hat{a} | \hat{b}^+ \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{e^{\beta\omega} + 1} A[(T_b^{-1})_{12}],$$

$$(T_b^{-1})_{12} = -\frac{T_{b12}}{T_{b11}} (T_b^{-1})_{22};$$

$$\langle \hat{c} | \hat{b}^+\hat{a} \rangle = \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{e^{\beta\omega} + 1} A[(T_c^{-1})_{21}],$$

$$(T_c^{-1})_{21} = -\frac{T_{c21}}{T_{c22}} (T_c^{-1})_{21}.$$

If  $\langle \hat{c} | \hat{b}^+\hat{a} \rangle$  is chosen to be used, it is first

necessary to evaluate

$$\begin{aligned}
 (T_C^{-1})_{21} &= \frac{\lambda_o \omega_o}{\omega + (\omega_o - \epsilon_o)} \\
 &\quad \times \left[ \frac{1}{\omega + \epsilon_o - \frac{(\lambda_o \omega_o)^2 (N_a + N_b)}{\omega + (\omega_o - \epsilon_o)}} \right] \\
 &= \lambda_o \omega_o \left[ \omega^2 + \omega \omega_o + \epsilon_o (\omega_o - \epsilon_o) \right. \\
 &\quad \left. - (\lambda_o \omega_o)^2 (N_a + N_b) \right]^{-1} \\
 &= \frac{\lambda_o \omega_o}{\omega^2 + a\omega + b} \\
 &= \lambda_o \omega_o \left[ \frac{c}{\omega + x} - \frac{d}{\omega + y} \right]
 \end{aligned}$$

using the following notation:

$$a = \omega_o,$$

$$b = \epsilon_o (\omega_o - \epsilon_o) - (\lambda_o \omega_o)^2 (N_a + N_b),$$

$$x = \frac{a}{2} \pm \left[ \left( \frac{a}{2} \right)^2 - b \right]^{1/2},$$

$$y = a - x,$$

$$c = d = \frac{1}{a - 2x}.$$

The corresponding spectral function is

$$A[T_C^{-1}]_{21} = i \lambda_o \omega_o \lim_{\delta \rightarrow 0} \left[ \left[ \frac{c}{\omega + i\delta + x} - \frac{c}{\omega - i\delta + x} \right] \right]$$

$$\begin{aligned}
& - \left[ \frac{d}{\omega + i\delta + y} - \frac{d}{\omega - i\delta + y} \right] \\
& = 2\lambda_0 \omega_0 \pi [\delta(\delta, \omega + x) - \delta(\delta, \omega + y)].
\end{aligned}$$

From this spectral function it is possible to calculate

$$\begin{aligned}
\langle \hat{a} \hat{b}^\dagger \hat{c} \rangle &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \frac{1}{e^{\beta\omega} + 1} A[(T_c^{-1})_{21}] \\
&= \lambda_0 \omega_0 \left[ \frac{1}{e^{-\beta x} + 1} - \frac{1}{e^{-\beta y} + 1} \right]
\end{aligned}$$

with

$$x = \frac{\omega_0}{2} + R,$$

$$y = \frac{\omega_0}{2} - R,$$

$$R = \left[ \left[ \frac{\omega_0}{2} \right]^2 - \epsilon_0 (\omega_0 - \epsilon_0) + (\lambda_0 \omega_0)^2 (N_a + N_b) \right]^{1/2}.$$

### 10.7. Evaluations for Thermodynamic Limits

When  $\lambda_0$  is finite, the equations for the different  $N_n$  are coupled. In general, the equations cannot be solved exactly. Certain limiting cases are exceptions. Some especially interesting ones are shown in Table 10.1.

The second-order solution for  $N_a$  in Table 10.1 is indeterminate in the limit of large temperature and in the limit of large coupling.

Table 10.1. Some limiting cases of expectation values.

	$\langle \hat{a} \hat{b} \hat{c} \rangle$	$N_a$	$N_b$	$N_c$
$T = 0$	0	0	$0^*$	$0^{**}$
$T \rightarrow \infty$	0	$1/\rho\omega_0$	1/2	1/2
$\lambda_0 \rightarrow 0$	0	$\frac{1}{e^{\beta\omega_0} - 1}$	$\frac{1}{e^{\beta\epsilon_0} + 1}$	$\frac{1}{e^{-\beta\epsilon_0} + 1}$
$\lambda_0 \rightarrow \infty$	$\lambda_0$	?	1/2	1/2

\* if  $\epsilon_0 > 0$

\*\* unless  $\epsilon_0 > 0$

## 11. Truncated Solution for Froehlich Model

### 11.1. Specification of Basis States

A particular variant of the Froehlich Hamiltonian operator is

$$\hat{H} = \sum_j \epsilon_j \hat{c}_j^\dagger \hat{c}_j + \sum_{k,p} M_p \hat{c}_{k+p}^\dagger \hat{c}_k (\hat{a}_p + \hat{a}_{-p}^\dagger) + \sum_p \omega_p \hat{a}_p^\dagger \hat{a}_p.$$

This Hamiltonian operator is complicated by summations over wave-vector states. In a physically realistic treatment, the subscript indices  $j, k, p$  would be tricomponent vectors  $\vec{j}, \vec{k}, \vec{p}$ . Because the purpose of the present exposition is the illustration of a technique, some realism is sacrificed for simplicity in the way the Hamiltonian operator is written. Even so, it does not appear that it is feasible to obtain an exact solution. In fact, it is not evident a priori that even a truncated analytical solution can be found.

By the now-familiar technique, the

$$\hat{L}\hat{\phi}_k = [\hat{\phi}_k, \hat{H}]$$

for basis states  $\hat{\phi}_k$  can be used to find matrix elements

$$T_{ki} = \frac{((\hat{\phi}_k, (\omega - \hat{L})\hat{\phi}_i))_c}{((\hat{\phi}_k, \hat{\phi}_k))_c}$$

that are then used to find the inverse-matrix elements

$$(T^{-1})_{lk} = \frac{((\hat{\phi}_1, (\omega - \hat{L})^{-1} \hat{\phi}_k))_c}{((\hat{\phi}_1, \hat{\phi}_1))_c}.$$

A sum of such inverse-matrix elements gives a Green function.

For a solution truncated to second order in the stepping operators, appropriate basis states are the following:

$$\hat{\phi}_{a1} = \hat{\phi}_1 = \hat{a}_q,$$

$$\hat{\phi}_{a2} = \hat{\phi}_2 = \hat{a}_{-q}^{\dagger},$$

$$\hat{\phi}_{c1} = \hat{\phi}_3 = \hat{c}_{k-q}^{\dagger} \hat{c}_k.$$

The boson states can be combined into a basis state

$$\hat{A}_q = \hat{a}_q + \hat{a}_{-q}^{\dagger}$$

that should lead to a Green function

$$((\hat{A}_q, (\omega - \hat{L})^{-1} \hat{A}_q))_c.$$

## 11.2. Proof Relating to Coupling Factor

The result of the following proof is needed:

$$\hat{H}_I = \sum_{k,p} M_p \hat{c}_{k+p}^{\dagger} \hat{c}_k (\hat{a}_p + \hat{a}_{-p}^{\dagger}),$$

$$\hat{H}_I^{\dagger} = \sum_{k,p} M_p^* \hat{c}_k^{\dagger} \hat{c}_{k+p} (\hat{a}_p^{\dagger} + \hat{a}_{-p}),$$

$$j \equiv k + p \Rightarrow j - p = k,$$

$$\hat{H}_I^+ = \sum_{k,p} M_p^* \hat{c}_{j-p}^+ \hat{c}_j (\hat{a}_{-p} + \hat{a}_p^+),$$

$$p = -p,$$

$$\begin{aligned} \hat{H}_I^+ &= \sum_{j,p} M_{-p}^* \hat{c}_{j+p}^+ \hat{c}_j (\hat{a}_p + \hat{a}_{-p}^+) \\ &= \sum_{k,p} M_{-p}^* \hat{c}_{k+p}^+ \hat{c}_k (\hat{a}_p + \hat{a}_{-p}^+), \end{aligned}$$

$$\hat{H}_I = \hat{H}_I^+,$$

$$\therefore M_p = M_{-p}^* = M_{-p},$$

$$\therefore M_q = M_{-q}.$$

### 11.3. Application of Liouville Superoperator

The Liouville superoperator acting on the basis states gives the following:

$$\hat{L}\hat{\Phi}_1 = \hat{L}\hat{a}_q = \omega_q \hat{a}_q + M_q \sum_k \hat{c}_{k-q}^+ \hat{c}_k,$$

$$\hat{L}\hat{\Phi}_2 = \hat{L}\hat{a}_{-q}^+ = -\omega_{-q} \hat{a}_{-q}^+ - M_{-q} \sum_k \hat{c}_{k-q}^+ \hat{c}_k,$$

$$\hat{L}\hat{A}_q = \omega_q (\hat{a}_q - \hat{a}_q^+),$$

$$\begin{aligned} \hat{L}\hat{\Phi}_3 &= \hat{L}\hat{c}_{k-q}^+ \hat{c}_k = (\epsilon_k - \epsilon_{k-q}) \hat{c}_{k-q}^+ \hat{c}_k \\ &\quad + \sum_p M_p (\hat{a}_p + \hat{a}_{-p}^+) \\ &\quad \times (\hat{c}_{k-q}^+ \hat{c}_{k-p} - \hat{c}_{k-q+p}^+ \hat{c}_k). \end{aligned}$$

## 11.4. Calculation of Inner Products

The inner products are as follows:

$$((\hat{\phi}_n, \hat{L}\hat{\phi}_n))_c = \langle [\hat{L}\hat{\phi}_n, \hat{\phi}_n^+] \rangle,$$

$$((\hat{\phi}_1, \hat{L}\hat{\phi}_1))_c = \omega_q,$$

$$((\hat{\phi}_1, \hat{L}\hat{\phi}_2))_c = 0,$$

$$\begin{aligned} ((\hat{\phi}_1, \hat{L}\hat{\phi}_3))_c &= \langle \sum_p M_p (\hat{c}_{k-q}^+ \hat{c}_{k-p} - \hat{c}_{k-q+p}^+ \hat{c}_k) \delta_{p,q} \rangle \\ &= M_q (N_{k-q} - N_k), \end{aligned}$$

$$((\hat{\phi}_2, \hat{L}\hat{\phi}_2))_c = \langle \omega_{-q} \rangle = \omega_q,$$

$$((\hat{\phi}_2, \hat{L}\hat{\phi}_3))_c = -M_q (N_{k-q} - N_k),$$

$$((\hat{\phi}_3, \hat{L}\hat{\phi}_1))_c = M_q (N_{k-q} - N_k),$$

$$((\hat{\phi}_3, \hat{L}\hat{\phi}_2))_c = -M_q (N_{k-q} - N_k),$$

$$((\hat{\phi}_3, \hat{L}\hat{\phi}_3))_c = (\epsilon_k - \epsilon_{k-q})(N_{k-q} - N_k) - S,$$

$$S \equiv - \langle \sum_p M_p \hat{A}_p (\hat{p}_{-p}^+ + \hat{p}_p) \rangle;$$

$$((\hat{\phi}_n, \hat{\phi}_n))_c = \langle [\hat{\phi}_n, \hat{\phi}_n^+] \rangle,$$

$$((\hat{\phi}_1, \hat{\phi}_1))_c = 1,$$

$$((\hat{\phi}_2, \hat{\phi}_2))_c = -1,$$

$$((\hat{\phi}_3, \hat{\phi}_3))_c = N_{k-q} - N_k,$$

$$((\hat{\phi}_2, \hat{\phi}_1))_c = 0.$$

### 11.5. Calculation of Resolvent Matrix Elements

The inner products are used to calculate the

$$T_{ki} = \delta_{ki} \omega - \frac{((\hat{\phi}_k, \hat{L}\hat{\phi}_i))_c}{((\hat{\phi}_k, \hat{\phi}_k))} :$$

$$T_{11} = \omega - \omega_q,$$

$$T_{12} = 0,$$

$$T_{13} = -M_q(N_{k-q} - N_k),$$

$$T_{21} = 0,$$

$$T_{22} = \omega + \omega_q,$$

$$T_{23} = -M_{-q}(N_{k-q} - N_k),$$

$$T_{31} = -M_{-q},$$

$$T_{32} = M_{-q},$$

$$T_{33} = \omega - (\epsilon_k - \epsilon_{k-q}) - S/(N_{k-q} - N_k).$$

### 11.6. Calculation of Matrix Elements

The simultaneous equations

$$\delta_{li} = \sum_k (T^{-1})_{lk} T_{ki}; \quad k = 1, 2, 3; \quad i = 1, 2, 3$$

can be solved to get the inverse-matrix elements:

$$(\mathbf{T}^{-1})_{11} = \left[ \mathbf{T}_{11} + \frac{\mathbf{T}_{13}(\mathbf{T}_{21}\mathbf{T}_{32} - \mathbf{T}_{22}\mathbf{T}_{31})}{\mathbf{T}_{21}\mathbf{T}_{33} - \mathbf{T}_{23}\mathbf{T}_{32}} + \frac{\mathbf{T}_{12}(\mathbf{T}_{23}\mathbf{T}_{31} - \mathbf{T}_{21}\mathbf{T}_{33})}{\mathbf{T}_{21}\mathbf{T}_{33} - \mathbf{T}_{23}\mathbf{T}_{32}} \right]^{-1},$$

$$(\mathbf{T}^{-1})_{12} = (\mathbf{T}^{-1})_{11} \left[ -\mathbf{T}_{12} + \frac{\mathbf{T}_{13}\mathbf{T}_{32}}{\mathbf{T}_{33}} \right] \times \left[ \mathbf{T}_{33} - \frac{\mathbf{T}_{32}\mathbf{T}_{23}}{\mathbf{T}_{22}} \right]^{-1},$$

$$(\mathbf{T}^{-1})_{22} = \left[ \mathbf{T}_{22} + \frac{\mathbf{T}_{21}(\mathbf{T}_{13}\mathbf{T}_{32} - \mathbf{T}_{12}\mathbf{T}_{33})}{\mathbf{T}_{11}\mathbf{T}_{33} - \mathbf{T}_{13}\mathbf{T}_{31}} + \frac{\mathbf{T}_{23}(\mathbf{T}_{12}\mathbf{T}_{31} - \mathbf{T}_{11}\mathbf{T}_{32})}{\mathbf{T}_{11}\mathbf{T}_{33} - \mathbf{T}_{13}\mathbf{T}_{31}} \right]^{-1},$$

$$(\mathbf{T}^{-1})_{21} = (\mathbf{T}^{-1})_{22} \left[ -\mathbf{T}_{21} + \frac{\mathbf{T}_{23}\mathbf{T}_{31}}{\mathbf{T}_{33}} \right] \times \left[ \mathbf{T}_{11} + \frac{\mathbf{T}_{13}\mathbf{T}_{31}}{\mathbf{T}_{33}} \right]^{-1},$$

$$(\mathbf{T}^{-1})_{23} = (\mathbf{T}^{-1})_{22} \left[ -\mathbf{T}_{23} + \frac{\mathbf{T}_{21}\mathbf{T}_{13}}{\mathbf{T}_{11}} \right] \times \left[ \mathbf{T}_{33} + \frac{\mathbf{T}_{31}\mathbf{T}_{13}}{\mathbf{T}_{11}} \right],$$

$$(\mathbf{T}^{-1})_{33} = \left[ \mathbf{T}_{33} + \frac{\mathbf{T}_{31}(\mathbf{T}_{12}\mathbf{T}_{23} - \mathbf{T}_{13}\mathbf{T}_{22})}{\mathbf{T}_{11}\mathbf{T}_{22} - \mathbf{T}_{12}\mathbf{T}_{21}} + \frac{\mathbf{T}_{32}(\mathbf{T}_{13}\mathbf{T}_{21} - \mathbf{T}_{11}\mathbf{T}_{23})}{\mathbf{T}_{11}\mathbf{T}_{22} - \mathbf{T}_{12}\mathbf{T}_{21}} \right]^{-1},$$

$$\begin{aligned}
(T^{-1})_{31} &= (T^{-1})_{33} \left[ -T_{31} + \frac{T_{32}T_{21}}{T_{22}} \right] \\
&\quad \times \left[ T_{11} + \frac{T_{12}T_{21}}{T_{22}} \right]^{-1},
\end{aligned}$$

$$\begin{aligned}
(T^{-1})_{32} &= (T^{-1})_{33} \left[ -T_{32} + \frac{T_{31}T_{12}}{T_{11}} \right] \\
&\quad \times \left[ T_{22} + \frac{T_{21}T_{12}}{T_{11}} \right]^{-1}.
\end{aligned}$$

Substitution of the particular expressions for the  $T_{ki}$  into the expressions for the  $(T^{-1})_{lk}$ , and use of the definitions

$$N \equiv N_{k-q} - N_k,$$

$$E \equiv \omega - (\epsilon_k - \epsilon_{k-q}) - S/N,$$

gives the following:

$$(T^{-1})_{11} = \left[ \omega - \omega_q - \frac{(\omega + \omega_q)}{\frac{(\omega + \omega_q)(\omega - E)}{M_q^2 N} + 1}} \right]^{-1},$$

$$(T^{-1})_{12} = -(T^{-1})_{11} \left[ \frac{(\omega + \omega_q)(\omega - E)}{M_q^2 N} + 1 \right]^{-1},$$

$$(T^{-1})_{13} = (T^{-1})_{11} \left[ \frac{\omega - E}{M_q N} + \frac{M_q}{\omega + \omega_q} \right]^{-1}.$$

$$(T^{-1})_{22} = \left[ \omega + \omega_q + \frac{(\omega - \omega_q)}{M_q^2 N} - 1 \right]^{-1},$$

$$(T^{-1})_{21} = (T^{-1})_{22} \left[ \frac{(\omega - \omega_q)(\omega - E)}{M_q^2 N} - 1 \right]^{-1},$$

$$(T^{-1})_{23} = (T^{-1})_{22} \left[ \frac{\omega - E}{M_q N} + \frac{M_q}{\omega - \omega_q} \right]^{-1},$$

$$(T^{-1})_{33} = \left[ \omega - E - \frac{M_q^2 N 2\omega_q}{(\omega^2 - \omega_q^2)} \right]^{-1},$$

$$(T^{-1})_{31} = (T^{-1})_{33} \left[ \frac{\omega - \omega_q}{M_q} \right]^{-1},$$

$$(T^{-1})_{32} = (T^{-1})_{33} \left[ \frac{\omega + \omega_q}{-M_q} \right]^{-1}.$$

### 11.7. Calculation of Green Function

Using the equation

$$R \equiv (\omega - L)^{-1},$$

it is possible to write the sought-after Green function as

$$\begin{aligned} & ((\hat{A}_q, (\omega - \hat{L})^{-1} \hat{A}_q)) \\ &= ((\hat{a}_q, R \hat{a}_q)) + ((\hat{a}_q, R \hat{a}_{-q}^*)) + ((\hat{a}_{-q}^*, R \hat{a}_q)) \\ &+ ((\hat{a}_{-q}^*, R \hat{a}_{-q}^*)) \\ &= [(T^{-1})_{11} + (T^{-1})_{12}] - [(T^{-1})_{21} + (T^{-1})_{22}]. \end{aligned}$$

The previously calculated expressions can be

substituted for the matrix elements to get the following expressions for the sums:

$$(T^{-1})_{11} + (T^{-1})_{12} = \frac{1}{(\omega - \omega_q) - \frac{M_q^2 N}{(\omega - E)}},$$

$$(T^{-1})_{22} + (T^{-1})_{21} = \frac{1}{(\omega + \omega_q) + \frac{M_q^2 N}{(\omega - E)}}.$$

The Green function can then be written as

$$\begin{aligned} & [(T^{-1})_{11} + (T^{-1})_{12}] - [(T^{-1})_{22} + (T^{-1})_{21}] \\ &= \frac{2\omega_{qk}}{\omega^2 - \omega_{qk}^2}, \end{aligned}$$

by using the following definition:

$$\omega_{qk} \equiv \omega_q + \frac{M_q^2 N}{(\omega - E)}.$$

### 11.8. Use of Summed Basis States

It is more realistic to assume that  $\hat{\phi}_3$  is a sum of basis states:

$$\hat{\phi}_3 = \sum_k \hat{c}_{k-q}^\dagger \hat{c}_k.$$

The Liouville superoperator gives

$$\hat{L}\hat{\phi}_3 = \sum_k (\epsilon_k - \epsilon_{k-q}) \hat{c}_{k-q}^\dagger \hat{c}_k + \sum_p M_p (\hat{a}_p + \hat{a}_{-p}^\dagger)$$

$$\times \left[ \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}-\mathbf{q}}^{\dagger} \hat{c}_{\mathbf{k}-\mathbf{p}} - \sum_{\mathbf{k}} \hat{c}_{\mathbf{k}-\mathbf{q}+\mathbf{p}}^{\dagger} \hat{c}_{\mathbf{k}} \right].$$

The inner products are the following:

$$((\hat{\phi}_1, \hat{L}\hat{\phi}_3))_c = M_q \sum_{\mathbf{k}} (N_{\mathbf{k}-\mathbf{q}} - N_{\mathbf{k}}),$$

$$((\hat{\phi}_3, \hat{L}\hat{\phi}_1))_c = M_{-q} \sum_{\mathbf{k}} (N_{\mathbf{k}-\mathbf{q}} - N_{\mathbf{k}}),$$

$$((\hat{\phi}_3, \hat{L}\hat{\phi}_3))_c = \sum_{\mathbf{k}} (\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}-\mathbf{q}}) (N_{\mathbf{k}-\mathbf{q}} - N_{\mathbf{k}}) \\ - \langle \sum_{\mathbf{p}} M_{\mathbf{p}} \hat{A}_{\mathbf{p}} (\hat{\rho}_{\mathbf{p}} + \hat{\rho}_{-\mathbf{p}}^{\dagger}) \rangle,$$

$$((\hat{\phi}_3, \hat{\phi}_3))_c = \sum_{\mathbf{k}} (N_{\mathbf{k}-\mathbf{q}} - N_{\mathbf{k}}),$$

$$((\hat{\phi}_3, \hat{L}\hat{\phi}_3))_c = -M_q \sum_{\mathbf{k}} (N_{\mathbf{k}-\mathbf{q}} - N_{\mathbf{k}}),$$

$$((\hat{\phi}_3, \hat{L}\hat{\phi}_2))_c = -M_{-q} \sum_{\mathbf{k}} (N_{\mathbf{k}-\mathbf{q}} - N_{\mathbf{k}}).$$

Note that some of these are neutral vectors:

$$\sum_{\mathbf{k}} (N_{\mathbf{k}-\mathbf{q}} - N_{\mathbf{k}}) = \sum_{\mathbf{j}} N_{\mathbf{j}} - \sum_{\mathbf{k}} N_{\mathbf{k}}.$$

Matrix elements are as follows:

$$T_{13} = -M_q N_s,$$

$$T_{23} = -M_q N_s,$$

$$T_{31} = -M_q,$$

$$T_{32} = M_q,$$

$$T_{33} = \omega - E_s.$$

The matrix elements are written in forms of the following definitions:

$$N_s \equiv \sum_k (N_{k-q} - N_k),$$

$$E_s \equiv \frac{\sum_k (\epsilon_k - \epsilon_{k-q}) N}{N_s} - \frac{S}{N_s}.$$

From the similarity of these expressions to the ones obtained using  $\hat{\phi}_3$ , it is apparent that the result is

$$((\hat{A}_q, (\omega - \hat{L})^{-1} \hat{A}_q)) = \frac{2\omega_{qs}}{\omega^2 - \omega_{qs}^2},$$

expressed in terms of

$$\omega_{qs} = \omega_q + \frac{M_q^2 N_s}{(\omega - E_s)}.$$

The flaw in this attempt to treat a multiplicity of  $\hat{\phi}_3$ -like basis states is that the solution involves division by norms of neutral vectors, and the norm of a neutral vector is zero.

### 11.9. Summed Basis States in Pontryagin Space

A way to handle a multiplicity of  $\hat{\phi}_3$ -type basis states in Pontryagin space is to rewrite the set of simultaneous equations

$$\delta_{1i} = \sum_k (T^{-1})_{1k} T_{ki}$$

as

$$\delta_{1i} = \sum_{j=1}^2 (T^{-1})_{1j} T_{ji} + \sum_k (T^{-1})_{1k} T_{ki} \delta_{ki}.$$

For the specific case under consideration, these simultaneous equations can be solved, after some algebraic manipulation, for the following inverse matrix elements:

$$\begin{aligned} (T^{-1})_{11} &= \left[ T_{11} - \sum_k \frac{T_{1k} T_{k1}}{T_{kk}} \right. \\ &\quad - \left[ T_{12} - \sum_k \frac{T_{1k} T_{k2}}{T_{22}} \right] \\ &\quad \times \left[ T_{21} - \sum_k \frac{T_{2k} T_{k1}}{T_{kk}} \right] \\ &\quad \left. \times \left[ T_{22} - \sum_k \frac{T_{2k} T_{k2}}{T_{kk}} \right]^{-1} \right]^{-1}, \end{aligned}$$

$$(T^{-1})_{12} = (T^{-1})_{11} \frac{\left[ -T_{12} + \sum_k \frac{T_{1k} T_{k2}}{T_{kk}} \right]}{\left[ T_{22} - \sum_k \frac{T_{2k} T_{k2}}{T_{kk}} \right]},$$

$$\begin{aligned} (T^{-1})_{22} &= \left[ T_{22} - \sum_k \frac{T_{2k} T_{k2}}{T_{kk}} \right. \\ &\quad - \left[ T_{21} - \sum_k \frac{T_{2k} T_{k1}}{T_{22}} \right] \end{aligned}$$

$$\begin{aligned}
& \times \left[ T_{12} - \sum_{\mathbf{k}} \frac{T_{1\mathbf{k}} T_{\mathbf{k}2}}{T_{\mathbf{k}\mathbf{k}}} \right] \\
& \times \left[ T_{11} - \sum_{\mathbf{k}} \frac{T_{1\mathbf{k}} T_{\mathbf{k}1}}{T_{\mathbf{k}\mathbf{k}}} \right]^{-1} \Big]^{-1}, \\
(T^{-1})_{21} &= (T^{-1})_{22} \frac{\left[ -T_{21} + \sum_{\mathbf{k}} \frac{T_{2\mathbf{k}} T_{\mathbf{k}1}}{T_{\mathbf{k}\mathbf{k}}} \right]}{\left[ T_{11} - \sum_{\mathbf{k}} \frac{T_{1\mathbf{k}} T_{\mathbf{k}1}}{T_{\mathbf{k}\mathbf{k}}} \right]}.
\end{aligned}$$

The Green function is

$$\begin{aligned}
& [(T^{-1})_{11} + (T^{-1})_{12}] - [(T^{-1})_{21} + (T^{-1})_{22}] \\
& = \frac{2\omega_{\mathbf{q}}}{\omega^2 - \omega_{\mathbf{q}}^2 - 2\omega_{\mathbf{q}} M_{\mathbf{q}}^2 \sum_{\mathbf{k}} \frac{N}{\omega - E}}.
\end{aligned}$$

## 12. Mahan's Independent Boson Model

### 12.1. Operator Similarity Transformations

An operator analog of a similarity transformation can transform a function of operators as follows:

$$\bar{f}(\hat{A}) = e^{\hat{S}} f(\hat{A}) e^{-\hat{S}}.$$

The transformation of a function of operators is the function of the transformed operators:

$$\begin{aligned} e^{\hat{S}} f(\hat{A}) e^{-\hat{S}} &= e^{\hat{S}} \sum_{n=0}^{\infty} a_n \hat{A}^n e^{-\hat{S}} \\ &= \sum_{n=0}^{\infty} a_n (\hat{A})^n \\ &= f(\hat{A}), \end{aligned}$$

$$e^{\hat{S}} \hat{A} e^{-\hat{S}} = e^{\hat{S}} \hat{A} e^{-\hat{S}} e^{\hat{S}} e^{-\hat{S}}.$$

On the basis of the preceding two statements, it is evident that particular operators in a transformed expression are individually subject to the transformation

$$\hat{A} = e^{\hat{S}} \hat{A} e^{-\hat{S}}.$$

Such a transformed operator can be evaluated by the expansion

$$e^{\hat{S}} \hat{A} e^{-\hat{S}} = \hat{A} + [\hat{S}, \hat{A}] + \frac{1}{2!} [\hat{S}, [\hat{S}, \hat{A}]] + \dots$$

(12.1)

## 12.2. Canonical Transformation of Hamiltonian

The Froehlich Hamiltonian operator

$$\hat{H} = \hat{c}^\dagger \hat{c} [\epsilon_c + \sum_q M_q (\hat{a}_q + \hat{a}_q^\dagger)] + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q \quad (12.2)$$

can be diagonalized (Mahan 1981) by a canonical transformation of the type

$$\begin{aligned} \hat{H} &= e^{\hat{s}} \hat{H} e^{-\hat{s}}, \\ \hat{s} &= \hat{c}^\dagger \hat{c} \sum_q \lambda_q (\hat{a}_q^\dagger - \hat{a}_q), \\ \lambda_q &= M_q / \omega_q. \end{aligned} \quad (12.3)$$

This is a unitary transformation with

$$\hat{s}^\dagger = -\hat{s}.$$

In writing the Hamiltonian operator and the transformation operator, use has been made of the relation

$$\sum_q M_q \hat{a}_{-q} = \sum_q M_q \hat{a}_q,$$

which follows from the already proven equivalence

$$M_q = M_{-q}.$$

For simplicity, the index for summation over boson wave-vector states has been chosen to be  $q$  rather than a vector  $\vec{q}$ .

The transform of the particular operator  $\hat{c}$  can be found by Eq. (12.1) and Eq. (12.3) to be

$$\hat{c} = \hat{c}\hat{X},$$

$$\hat{X} = \exp\left[-\sum_q \lambda_q (\hat{a}_q^\dagger - \hat{a}_q)\right].$$

The transformed Hamiltonian operator contains the product

$$\begin{aligned} \hat{c}^\dagger \hat{c} &= \hat{X}^\dagger \hat{c}^\dagger \hat{c} \hat{X} \\ &= \hat{c}^\dagger \hat{c} \hat{X}^\dagger \hat{X} \\ &= \hat{c}^\dagger \hat{c} \hat{X}^{-1} \hat{X} \\ &= \hat{c}^\dagger \hat{c}. \end{aligned} \tag{12.4}$$

The transform of the particular operator  $\hat{a}$  is found by Eq. (12.1) and Eq. (12.3) to be

$$\hat{a} = \hat{a} - \lambda_q \hat{c}^\dagger \hat{c}. \tag{12.5}$$

The substitution of Eq. (12.4) and Eq. (12.5) into Eq. (12.2) determines the transformed Hamiltonian operator

$$\begin{aligned} \hat{H} &= \epsilon_c \hat{c}^\dagger \hat{c} + \hat{c}^\dagger \hat{c} \sum_q M_q (\hat{a}_q + \hat{a}_q^\dagger) + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q \\ &= \epsilon_c \hat{c}^\dagger \hat{c} + \hat{c}^\dagger \hat{c} \sum_q M_q (\hat{a} + \hat{a}^\dagger - 2\lambda_q \hat{c}^\dagger \hat{c}) \\ &\quad + \sum_q \omega_q (\hat{a}_q^\dagger - \lambda_q \hat{c}^\dagger \hat{c}) (\hat{a}_q - \lambda_q \hat{c}^\dagger \hat{c}) \\ &= \hat{c}^\dagger \hat{c} (\epsilon_c - \Delta) + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q, \end{aligned}$$

$$\Delta \equiv \sum_{\mathbf{q}} M_{\mathbf{q}} \lambda_{\mathbf{q}}. \quad (12.6)$$

### 12.3. Green Function

In Sec. 7.1 it was explained that a Green function of two operators  $\hat{A}$  and  $\hat{B}^\dagger$  can be written as

$$\begin{aligned} G(t) &= -i\theta(t) \langle [\hat{A}(t), \hat{B}^\dagger(0)] \rangle \\ &= -i\theta(t) \text{Tr}[\hat{\rho} \hat{A}(t), \hat{B}^\dagger(0)]. \end{aligned}$$

The Green function

$$\begin{aligned} G(k, t) &= -i\theta(t) \langle \{\hat{c}(t), \hat{c}^\dagger(0)\} \rangle \\ &= -i\theta(t) \text{Tr}[\hat{\rho} \hat{c}(t) \hat{c}^\dagger(0)] \\ &= -i\theta(t) \text{Tr}(\hat{\rho} e^{i\hat{H}t} \hat{c} e^{-i\hat{H}t} \hat{c}^\dagger) \\ &= -i\theta(t) \text{Tr}(\hat{\rho} e^{i\hat{H}t} \hat{c} e^{-i\hat{H}t} \hat{c}^\dagger e^{\hat{s}} e^{-\hat{s}}). \end{aligned}$$

The cyclic properties of the trace allow this to be rewritten as

$$\begin{aligned} G(t) &= -i\theta(t) \text{Tr}(e^{\hat{s}} \hat{\rho} e^{i\hat{H}t} \hat{c} e^{-i\hat{H}t} \hat{c}^\dagger e^{-\hat{s}}) \\ &= -i\theta(t) \text{Tr}(\hat{\rho} e^{i\hat{H}t} \hat{c} e^{-i\hat{H}t} \hat{c}^\dagger) \\ &= -i\theta(t) \text{Tr}(\hat{\rho} e^{i\hat{H}t} \hat{c} \hat{X} e^{-i\hat{H}t} \hat{X}^\dagger \hat{c}^\dagger) \\ &= -i\theta(t) \text{Tr}(\hat{\rho} e^{i\hat{H}t} \hat{c} \hat{X} e^{-i\hat{H}t} \hat{c}^\dagger \hat{X}^\dagger). \end{aligned}$$

Because the transformed Hamiltonian operator is diagonal in  $\hat{c}$  and  $\hat{a}$ , it is possible to prove the relation

$$e^{i\hat{H}t} \hat{c}^\dagger e^{-i\hat{H}t} = e^{-it(\epsilon_c - \Delta)} \hat{c}^\dagger(t),$$

$$\hat{X}(t) = \exp \left[ -\sum_q \lambda_q (\hat{a}_q^\dagger e^{i\omega_q t} - \hat{a}_q e^{-i\omega_q t}) \right]. \quad (12.7)$$

Substitution of the expressions

$$\frac{\hat{\rho}}{\rho} = e^{-\beta(\bar{H} - \Omega)},$$

$$\bar{\epsilon}_c \equiv \epsilon_c - \Delta,$$

as well as Eq. (12.6) and Eq. (12.7), into the expression for the Green function gives

$$G(t) = -i\theta(t) e^{\beta\Omega} \text{Tr} \left[ \left[ \exp \left[ -\beta \left[ \hat{c}^\dagger \hat{c} \bar{\epsilon}_c + \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q \right] \right] \right] \right. \\ \left. \times e^{-it\bar{\epsilon}_c} \hat{c}^\dagger \hat{c} \hat{X}(t) \hat{X}^\dagger(0) \right].$$

The boson and fermion parts can be collected into separate factors to give

$$G(t) = -i\theta(t) e^{\beta\Omega} \text{Tr} \left[ e^{-\beta \hat{c}^\dagger \hat{c} \bar{\epsilon}_c} \hat{c}^\dagger \hat{c} e^{-it\bar{\epsilon}_c} \right] \\ \times e^{\beta\Omega} \text{Tr} \left[ \left[ \exp \left[ -\beta \sum_q \omega_q \hat{a}_q^\dagger \hat{a}_q \right] \right] \hat{X}(t) \hat{X}^\dagger(0) \right].$$

The fermion part can be evaluated to give (Mahan 1981)

$$e^{\beta\Omega} \text{Tr} \left[ e^{-\beta \hat{c}^\dagger \hat{c} \bar{\epsilon}_c} \hat{c}^\dagger \hat{c} e^{-it\bar{\epsilon}_c} \hat{c}^\dagger \hat{c} e^{-it\bar{\epsilon}_c} \right] \\ = e^{-it\bar{\epsilon}_c} [1 - \langle \hat{c}^\dagger \hat{c} \rangle].$$

The boson part is evaluated by the use of

$$\overline{\prod_{\mathbf{q}} e^{f(\mathbf{q})}} = \exp \sum_{\mathbf{q}} f(\mathbf{q}),$$

and Feynman's theorem on the disentangling of operators.

#### 12.4. Boson Factors

A different approach towards attempting to evaluate the boson part is taken here. In the boson part, the first factor inside the trace is an exponential involving normally ordered boson stepping operators, with the creation operator appearing to the left of the annihilation operator. The other factors in the trace can be expanded in terms of sums of products of boson stepping operators. It would be desirable to write the expansions so that the products of boson stepping operators in the sums are normally ordered, with all creation operators in a term of a sum appearing to the left of all annihilation operators in that term of the sum. Sums that are normally ordered in this way have been found to have very significant convergence properties (Cahill and Glauber 1969).

Individual fermion excitations of the Hamiltonian operator can be examined through the time dependence of

$$\begin{aligned} \hat{c}(t) &= e^{i\hat{H}t} \hat{c} e^{-i\hat{H}t} \\ &= e^{-i(\epsilon_c - \Delta)t} \hat{c}(t), \end{aligned}$$

which can be evaluated only if  $\hat{X}(t)$ , containing the boson factors, can be determined.

### 12.5. Displacement Operator

A simplification of the Froehlich Hamiltonian is the Einstein model, which has a single boson mode, with no summation over the  $q$  index. For purposes of exposition, this simplification facilitates the study of  $\hat{X}(t)$ , which reduces to

$$\hat{X}(t) = \exp[-\lambda_0 (\hat{a}^\dagger e^{i\omega_0 t} - \hat{a} e^{-i\omega_0 t})].$$

Incidentally, it is possible to relate this to the unitary exponential displacement operator

$$\hat{D}(z) \equiv \exp[z(\hat{a}^\dagger - \hat{a})]$$

by the equation

$$\hat{X}(0) = \hat{D}(-\lambda_0).$$

### 12.6. Campbell-Baker-Hausdorff Theorem

So far in this exposition, exponentials involving operators generally have been expanded as series before further algebraic manipulations were performed on them. When it is desirable to work with the exponentials as such, and to manipulate them directly, it is necessary to continue to pay attention to the fact that operators are involved.

One relevant and significant relation, known as the Campbell-Baker-Hausdorff theorem (Douglas 1982), states

that, if the commutator  $[\hat{A}, \hat{B}]$  of two operators  $\hat{A}$  and  $\hat{B}$  commutes with both  $\hat{A}$  and  $\hat{B}$ , then (Mahan 1981)

$$e^{\hat{A} + \hat{B}} = e^{\hat{A}} e^{\hat{B}} e^{-1/2[\hat{A}, \hat{B}]}$$

Applying this relation gives

$$\hat{X}(t) = e^{-\lambda_0^2/2} \exp(-\lambda_0 \hat{a}^\dagger e^{i\omega_0 t}) \exp(\lambda_0 \hat{a} e^{-i\omega_0 t})$$

### 12.7. Expansion of Boson Factor

It is now possible to proceed with the expansion of

$$\begin{aligned} \hat{X}(t) &= e^{-\lambda_0^2/2} [-\lambda_0 (\hat{a} e^{-i\omega_0 t})^\dagger] \exp[\lambda_0 (\hat{a} e^{-i\omega_0 t})] \\ &= e^{-\lambda_0^2/2} \sum_{l=0}^{\infty} \frac{(-1)^l \lambda_0^l}{l!} [(\hat{a} e^{-i\omega_0 t})^\dagger]^l \\ &\quad \times \sum_{m=0}^{\infty} \frac{\lambda_0^m}{m!} (\hat{a} e^{-i\omega_0 t})^m \\ &= e^{-\lambda_0^2/2} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^l \lambda_0^{l+m}}{l!m!} (\hat{a}^\dagger)^l \hat{a}^m e^{i(1-m)\omega_0 t} \end{aligned}$$

### 12.8. Rearrangement of Double Sum

The double sum now consists of terms involving products of normally ordered stepping operators, but the creation and annihilation operators in a term are not raised to the same power. To proceed further, it is necessary to examine the relation of the range of the index of one sum to the range of the index of the other sum. One of two ways to express

these relations is as follows:

$$n = m - 1,$$

$$m = n + 1,$$

$$l = m - n.$$

With the assistance of these relations, it is possible to proceed with the rewriting of

$$\begin{aligned} \hat{X}(t) &= e^{-\lambda^2/2} \sum_{l=0}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^l \lambda_o^{2l+n} (\hat{a}^+)^{l^{\wedge}1+n} e^{-in\omega_o t}}{l!(n+1)!} \\ &+ e^{-\lambda^2/2} \sum_{n=-1}^{\infty} \sum_{m=0}^{\infty} \frac{(-1)^{m-n} \lambda_o^{2m-n} (\hat{a}^+)^{m-n} \hat{a}^m}{(m-n)!m!} \\ &\quad \times e^{-in\omega_o t} \\ &= e^{-\lambda^2/2} \sum_{n=0}^{\infty} \left[ \sum_{l=0}^{\infty} \frac{(-1)^l \lambda_o^{n+2l} (\hat{a}^+)^{l^{\wedge}1}}{l!(n+1)!} \right] \\ &\quad \times (\hat{a} e^{-i\omega_o t})^n \\ &+ e^{-\lambda^2/2} \sum_{n=1}^{\infty} \left[ \left[ -e^{i\omega_o t} \hat{a}^+ \right]^+ \right]^n \\ &\quad \times \sum_{m=0}^{\infty} \frac{(-1)^m (\lambda_o^+)^{n+2m} (\hat{a}^+)^m \hat{a}^m}{m!(n+m)!}. \end{aligned}$$

It happens that it is possible to write this as

$$\hat{X}(t) = \hat{g}(2\lambda_o, t),$$

which is the generating function of a novel mathematical

construct that can be regarded as a sort of generalized operator-valued Bessel function.

### 13. Generalized Bessel Functions

#### 13.1. Definition

It is convenient to define two new operators. One of these is

$$\hat{t} \equiv \hat{a} e^{-i\omega_0 t}.$$

The other is a new mathematical construct that might be considered to be a generalized operator-valued Bessel function of integer order defined by

$$\hat{J}_n(2z) \equiv \sum_{s=0}^{\infty} \frac{(-1)^s z^{n+2s} (\hat{a}^+)^s \hat{a}^s}{s!(n+s)!}.$$

It is immediately apparent that

$$\hat{J}_n^+(2z) = \hat{J}_n(2z).$$

#### 13.2. Generating Function

The generating function for Bessel function  $J_n(2z)$  is

$$\begin{aligned} g(2z, t) &= e^{z(t-1/t)} \\ &= \sum_{n=-\infty}^{\infty} J_n(2z) t^n \\ &= J_0(2z) + \sum_{n=1}^{\infty} \left[ J_n(2z) t^n + \left[ \frac{-1}{t} \right]^n J_n(2z) \right]. \end{aligned}$$

An analogous generating function for the generalized Bessel function  $\hat{J}_n(2z)$  is

$$\begin{aligned}\hat{g}(2z, \hat{t}) &= e^{z(\hat{t}-\hat{t}^*)} \\ &= e^{-z^2/2} \left[ \hat{J}_0(2z) + \sum_{n=1}^{\infty} \left[ \hat{J}_n(2z) \hat{t}^n \right. \right. \\ &\quad \left. \left. + (-\hat{t}^*)^n \hat{J}_n(2z) \right] \right].\end{aligned}$$

The prefactor appears as a result of the Campbell-Baker-Hausdorff theorem.

Thus it turns out that this last generating function has the same form as, and can be used to represent,

$$\hat{X}(t) = \hat{g}(2\lambda_0, \hat{t}).$$

### 13.3. Simple properties

Some of the simple relations for Bessel functions, such as

$$J_n(2z) = J_n^*(2z),$$

$$J_n(2z) = (-1)^n J_n(-2z),$$

$$J_n(2z) = (-1)^n J_{-n}(2z),$$

have almost identical parallels for the generalized Bessel functions:

$$\hat{J}_n(2z) = \hat{J}_n^+(2z),$$

$$\hat{J}_n(2z) = (-1)^n \hat{J}_n^+(-2z),$$

$$\hat{J}_n(2z) = (-1)^n \hat{J}_{-n}^+(2z).$$

#### 13.4. Recursion Relations

A recursion relation for the Bessel functions such as

$$1 = [J_0(2z)]^2 + 2 \sum_{n=1}^{\infty} [J_n(2z)]^2$$

has a corresponding relation for the generalized Bessel functions that is more complicated:

$$1 = e^{-z^2} \left[ [\hat{J}_0(2z)]^2 + \sum_{n=1}^{\infty} \hat{J}_n(2z) (\hat{a}^+)^n a^n \hat{J}_n(2z) + \sum_{n=1}^{\infty} (\hat{a}^+)^n \hat{J}_n(-2z) \hat{J}_n(-2z) \hat{a}^n \right].$$

A differential recursion relation for Bessel functions is (Watson 1952; Whittaker and Watson 1962; Arfken 1970)

$$z^n \frac{d}{dz} [z^{-n} J_n(2z)] = -2J_{n+1}(2z).$$

A corresponding differential recursion relation for the generalized Bessel functions is more complicated:

$$\begin{aligned} z^n \frac{d}{dz} [z^{-n} \hat{J}_n(2z)] &= \sum_{s=0}^{\infty} \frac{(-1)^s 2^s z^{n+2s-1} (\hat{a}^+)^s a^s}{s!(n+s)!} \\ &= \sum_{s=0}^{\infty} \frac{(-1)^s 2^s z^{n+2s-1} (\hat{a}^+)^s a^s}{(s-1)!(n+s)!} \end{aligned}$$

$$\begin{aligned}
&= -2\hat{a}^+ \sum_{s=0}^{\infty} \frac{(-1)^{s+1} z^{n+2(s-1)} (\hat{a}^+)^{s-1} \hat{a}^{s-1}}{(s-1)!(m+s-1)!} \\
&= -2\hat{a}^+ \sum_{s=0}^{\infty} \frac{(-1)^r z^{m+2r} (\hat{a}^+)^r \hat{a}^r}{r!(m+r)!} \\
&= -2\hat{a}^+ \hat{J}_{n+1}(2z)\hat{a};
\end{aligned}$$

$$\therefore z^{n+1} \frac{d}{dz} [z^{-n} \hat{J}_n(2z)] = -2\hat{a}^+ z \hat{J}_{n+1}(2z)\hat{a}.$$

This can be further simplified:

$$\begin{aligned}
&\hat{a}^+ z \hat{J}_{n+1}(2z)\hat{a} \\
&= - \sum_{r=0}^{\infty} \frac{(-1)^r z^{n+2r} (\hat{a}^+)^r \hat{a}^r}{r!(n+r)!} \\
&\quad - \sum_{r=0}^{\infty} \frac{(-1)^r z^{n+2r} (\hat{a}^+)^r \hat{a}^r}{r!(n+r-1)!} \\
&= n \hat{J}_n(2z) - z \hat{J}_{n-1}(2z).
\end{aligned}$$

### 13.5. Commutation Relations

A useful commutation relation for boson stepping operators is

$$[\hat{a}^q, (\hat{a}^+)^p \hat{a}^p] = \sum_{j=1}^{\infty} \begin{bmatrix} p \\ q \end{bmatrix} \begin{bmatrix} q \\ j \end{bmatrix} j! (\hat{a}^+)^{p-j} \hat{a}^{r+q-j}.$$

This relation can be used to get commutation relations involving the generalized Bessel functions.

In this relation, the infinite sum over the index  $j$  is terminated at the lesser of  $q$  and  $p$  by the  $(q-j)!$  or  $(p-j)!$  terms in the denominators of the binomial

coefficients because these factorials make terms in the sum vanish for  $q < j$  and  $p < j$ , respectively. A similar sort of termination of terms, brought about by a factorial or factorials in the denominators, is a typical feature of sums used to express commutation relations involving boson stepping operators. This sort of termination prevents the appearance of stepping operators with negative exponents.

Another simple example of a commutation relation expressed as a sum of products of boson stepping operators is

$$[\hat{D}(z), \hat{a}^p] = \sum_{j=1}^p \begin{bmatrix} p \\ j \end{bmatrix} (-z)^j (\hat{a}^+)^{p-j} \hat{D}(z).$$

A somewhat more complicated example is the relation

$$\begin{aligned} [\hat{a}^q, \hat{J}_n(2z)] &= \sum_{s=0}^{\infty} \frac{(-1)^s z^{n+2s}}{s!(n+s)!} [\hat{a}^a, (\hat{a}^+)^s \hat{a}^s] \\ &= \sum_{s=0}^{\infty} \frac{(-1)^s z^{n+2s}}{s!(n+s)!} \\ &\quad \times \sum_{j=1}^{\infty} \frac{q! s! (\hat{a}^+)^{s-j} \hat{a}^{s-j} \hat{a}^q}{(q-j)!(s-j)!j!} \\ &= \sum_{j=1}^{\infty} (-1)^j z^j \begin{bmatrix} q \\ j \end{bmatrix} \hat{J}_{n+j}(2z) \hat{a}^q \\ &= \sum_{j=1}^{\infty} (-1)^j z^j \begin{bmatrix} q \\ j \end{bmatrix} \hat{J}_{n+q}(2z) \hat{a}^q. \end{aligned}$$

An even more complicated example is the relation

$$\begin{aligned}
& [\hat{J}_n(2z), \hat{D}(z)] \\
&= \sum_{s=0}^{\infty} \frac{(-1)^s z^{n+2s}}{s!(n+s)!} [(\hat{a}^+)^s \hat{a}^s, \hat{D}(z)] \\
&= \sum_{j=1}^{\infty} \frac{(-1)^{j+1} z^j}{j!} (\hat{a}^+)^j \sum_{s=0}^{\infty} \frac{(-1)^s z^{n+2s} (\hat{a}^+)^{s-j} \hat{a}^{2-j} \hat{D}(z)}{(s-j)!(n+s)!} \\
&\quad + \sum_{j=1}^{\infty} \frac{(-1)^{j+1} z^j}{j!} \sum_{s=0}^{\infty} \frac{(-1)^s z^{n+2s} (\hat{a}^+)^{s-j} \hat{a}^{2-j} \hat{a}^j \hat{D}(z)}{(s-j)!(n+s)!}.
\end{aligned}$$

This example can be simplified by making the substitution:

$$\begin{aligned}
& \sum_{s=0}^{\infty} \frac{(-1)^s z^{n+2s} (\hat{a}^+)^{s-j} \hat{a}^{s-j}}{(s-j)!(n+s)!} \\
&= \sum_{t=0}^{\infty} \frac{(-1)^{t+j} z^{n+2t+2j} (\hat{a}^+)^t \hat{a}^t}{t!(n+t+j)!} \\
&= z^j \sum_{s=0}^{\infty} \frac{(-1)^{t+j} z^{(n+j)+2t} (\hat{a}^+)^t \hat{a}^t}{(s-j)!(n+s)!} \\
&= (-z)^j \hat{J}_{n+j}(2z).
\end{aligned}$$

With this substitution, the example reduces to

$$\begin{aligned}
& [\hat{D}(z), \hat{J}_n(2z)] \\
&= - \sum_{j=1}^{\infty} \frac{z^{2j}}{j!} [(\hat{a}^+)^j \hat{J}_{n+j}(2z) + \hat{J}_{n+j}(2z) \hat{a}^j] \hat{D}(z).
\end{aligned}$$

### 13.6. Miscellaneous Properties

Some miscellaneous relations that are useful in calculating with boson stepping operators are the following:

$$\hat{a}^n \hat{a}^+ = n \hat{a}^{n-1} + \hat{a}^+ \hat{a}^n,$$

$$\hat{a} (\hat{a}^+)^n = n (\hat{a}^+)^{n-1} + (\hat{a}^+)^n \hat{a},$$

$$\hat{a} \hat{J}_n(2z) = \hat{J}_n(2z) \hat{a} - z \hat{J}_{n+1}(2z) \hat{a},$$

$$\hat{J}_n(2z) \hat{a}^+ = \hat{a}^+ \hat{J}_n(2z) - z \hat{a}^+ \hat{J}_{n+1}(2z),$$

$$z \hat{a}^+ \hat{J}_{n+1}(2z) \hat{a} = n \hat{J}_n(2z) - z \hat{J}_{n-1}(2z),$$

$$\begin{aligned} \hat{a} \hat{a}^+ \hat{J}_n(2z) &= n (\hat{a}^+)^{n-1} \hat{J}_n(2z) + (\hat{a}^+)^n \hat{J}_n(2z) \hat{a} \\ &\quad - z (\hat{a}^+)^n \hat{J}_{n+1}(2z) \hat{a}. \end{aligned}$$

## 14. Simple Boson Factors

### 14.1. Displaced Harmonic Oscillator

The Hamiltonian for a displaced harmonic oscillator, expressed in second-quantized form, is (Haken 1976:41)

$$\hat{H} = \hbar\omega_0 \hat{a}^\dagger \hat{a} - \lambda_0 \hbar\omega_0 (\hat{a} + \hat{a}^\dagger).$$

As is evident from the relation (Mahan 1981:6)

$$x = \left[ \frac{\hbar}{2m\omega_0} (\hat{a} + \hat{a}^\dagger) \right]^{1/2},$$

the terms linear in the stepping operators represent the displacement. The eigenvalues are (Haken 1976:43)

$$E_n = n\hbar\omega_0 - \hbar\omega_0 \lambda_0^2.$$

The zero-point energy  $\hbar\omega_0/2$  has been ignored here. The eigenfunctions can be written in terms of the ground state as (Haken 1976:47)

$$\psi = \frac{\hat{D} (\hat{a}^\dagger)^n}{\sqrt{n!}} \psi_0,$$

where  $\hat{D}$  is the unitary exponential displacement operator.

### 14.2. Use of Displacement Operator

Fermion-boson Hamiltonian operators often contain displacement terms, such as appear in the Hamiltonian operator describing the displaced harmonic oscillator. Therefore it seems reasonable to suppose that the basis

states associated with a Hamiltonian operator or Liouville superoperator containing displacement terms should involve the unitary exponential displacement operator

$$\hat{D} = \hat{D}(\lambda_0).$$

From the exponential expansion of the exponential displacement operator, get

$$[\hat{D}, \hat{a}^\dagger \hat{a}] = -\lambda_0 (\hat{D} \hat{a} + \hat{a}^\dagger \hat{D}). \quad (14.1)$$

Substitute

$$\hat{a}^\dagger \hat{D} = \hat{D} \hat{a}^\dagger + \lambda_0 \hat{D}$$

into Eq. (14.1) to get

$$[\hat{D}, \hat{a}^\dagger \hat{a}] = -\lambda_0 \hat{D} (\hat{a} + \hat{a}^\dagger) - \lambda_0^2 \omega_0 \hat{D}. \quad (14.2)$$

Substitute

$$\hat{D} \hat{a} = \hat{a} \hat{D} - \lambda_0 \hat{D}$$

into Eq. (14.1) to get

$$[\hat{D}, \hat{a}^\dagger \hat{a}] = -\lambda_0 (\hat{a} + \hat{a}^\dagger) \hat{D} + \lambda_0^2 \omega_0 \hat{D}. \quad (14.3)$$

Recall the relation

$$[\hat{a}^n, \hat{a}^\dagger \hat{a}] = n \hat{a}^n. \quad (14.4)$$

With these substitutions, it is possible to evaluate the commutator of the boson number operator with a boson operator  $\hat{B}$  of certain forms.

For

$$\hat{B} = \hat{A} \hat{a}^n \hat{D}$$

use Eq. (14.2) and Eq. (14.4) to calculate

$$\begin{aligned} \omega_0[\hat{B}, \hat{a}^+ \hat{a}] &= \omega_0[\hat{A}, \hat{a}^+ \hat{a}] \hat{a}^n \hat{D} \\ &\quad + \hat{A} \hat{a}^n \omega_0[\hat{D}, \hat{a}^+ \hat{a}] \\ &\quad + \omega_0 \hat{A}[\hat{a}^n, \hat{a}^+ \hat{a}] \hat{D} \\ &= \omega_0[\hat{A}, \hat{a}^+ \hat{a}] \hat{a}^n \hat{D} + (n\omega_0 - \lambda_0^2 \omega_0) \hat{B} \\ &\quad - \lambda_0 \omega_0 \hat{B}(\hat{a} + \hat{a}^+). \end{aligned} \quad (14.5)$$

For

$$\hat{B} = \hat{D} \hat{a}^n \hat{A}$$

use Eq. (14.3) and Eq. (14.4) to calculate

$$\begin{aligned} \omega_0[\hat{B}, \hat{a}^+ \hat{a}] &= \omega_0 \hat{D} \hat{a}^n [\hat{A}, \hat{a}^+ \hat{a}] \\ &\quad + \omega_0 \hat{D}[\hat{a}^n, \hat{a}^+ \hat{a}] \hat{A} \\ &\quad + \omega_0[\hat{D}, \hat{a}^+ \hat{a}] \hat{a}^n \hat{A} \\ &= \omega_0 \hat{D} \hat{a}^n [\hat{A}, \hat{a}^+ \hat{a}] + (n\omega_0 - \lambda_0^2 \omega_0) \hat{B} \\ &\quad - \lambda_0 \omega_0 (\hat{a} + \hat{a}^+) \hat{B}. \end{aligned} \quad (14.6)$$

The first term on the right-hand sides of Eq. (14.5) and (14.6) vanishes if

$$[\hat{A}, \hat{a}^+ \hat{a}] = 0.$$

### 14.3. Boson Subfactors

What should  $\hat{A}$  be in order that its commutator with the boson number operator should vanish? The simplest possibility is that it is a constant. If  $\hat{A}$  were zero, the eigenfunction would also be zero. This would be a trivial case. If  $\hat{A}$  were a non-zero constant, if  $\hat{\Psi}$  were a product of a fermion factor  $\hat{F}$  and a boson factor  $\hat{B}$ , and if  $\hat{B}$  were a product of subfactors  $\hat{A}$  and  $\hat{S}$ , then the eigenvalue equation

$$\hat{L}\hat{\Psi} = F\hat{\Psi}$$

could be written as

$$\hat{L}\hat{F}\hat{A}\hat{S} = F\hat{F}\hat{A}\hat{S}$$

or as

$$\hat{L}\hat{F}\hat{S} = F\hat{F}\hat{S},$$

so that the  $\hat{A}$  would have the same effect as unity. The conclusion, therefore is that the simplest possibility for  $\hat{A}$  is that it is unity.

Another possibility for  $\hat{A}$  is that it is a generalized Bessel function, because

$$[\hat{J}_n(2\lambda_0), \hat{a}^+\hat{a}] = 0.$$

Of course, there are other boson subfactors that commute with the boson number operator. One of these will now be found.

Construct a stepping operator, as a product of factors,

in Judd form:

$$\hat{\phi}_{1m} = \hat{A}_1^\dagger \hat{I}_e \hat{A}_m.$$

This form contains the projection operator for the grand vacuum, so that

$$\hat{I}_e |0, 0\rangle = |0, 0\rangle.$$

The notation indicates that the ket is a zero state for both fermions and bosons. The factor

$$\hat{I}_e = \hat{I}_F \hat{I}_B$$

is a product of a fermion subfactor and a boson subfactor.

The boson subfactor is the projection operator

$$\hat{I}_B = |0\rangle\langle 0|.$$

The fermion subfactor is simply

$$\hat{I}_F = \hat{F}\hat{F}^\dagger.$$

The other factors are

$$\hat{A}_1^\dagger = \frac{(\hat{a}^\dagger)^1}{\sqrt{1!}},$$

$$\hat{A}_m = \frac{\hat{a}^m}{\sqrt{m!}}.$$

Use

$$|1\rangle = \frac{(\hat{a}^\dagger)^1}{\sqrt{1!}} |0\rangle,$$

$$\langle m | = \frac{\langle 0 | \hat{a}^m}{\sqrt{m!}},$$

to form

$$\begin{aligned} \hat{P}(1, m) &= |1\rangle \langle m| \\ &= \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle \langle 0| \frac{\hat{a}^m}{\sqrt{m!}} \end{aligned}$$

and calculate

$$\begin{aligned} [P(1, m), \hat{a}^+ \hat{a}] &= \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle \langle 0| \frac{\hat{a}^m}{\sqrt{m!}} \hat{a}^+ \hat{a} \\ &\quad - \hat{a}^+ \hat{a} \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle \langle 0| \frac{\hat{a}^m}{\sqrt{m!}} \\ &= \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle \langle 0| (m \hat{a}^{m-1} + \hat{a}^+ \hat{a}^m) \frac{\hat{a}}{\sqrt{m!}} \\ &\quad - \frac{(\hat{a}^+)^1}{\sqrt{1!}} [1(\hat{a}^+)^{1-1} \\ &\quad + (\hat{a}^+)^1 \hat{a}] |0\rangle \langle 0| \frac{\hat{a}^m}{\sqrt{m!}} \\ &= \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle \langle 0| \frac{\hat{a}^m}{\sqrt{m!}} m \\ &\quad - \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle \langle 0| \frac{\hat{a}^m}{\sqrt{m!}} 1 \\ &= (m - 1) \hat{P}(1, m). \end{aligned} \tag{14.7}$$

Note the special case

$$[\hat{P}(1, 1), \hat{a}^+ \hat{a}] = 0.$$

For

$$n \equiv m - 1,$$

get

$$\begin{aligned} \hat{P}(1, m) &= \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle\langle 0| \frac{\hat{a}^m}{\sqrt{m!}} \\ &= \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle\langle 0| \frac{\hat{a}^{1+n}}{\sqrt{(1+n)!}} \\ &= \frac{(\hat{a}^+)^1}{\sqrt{1!}} |0\rangle\langle 0| \frac{\hat{a}^1}{\sqrt{1!}} \frac{\sqrt{1!}}{\sqrt{(1+n)!}} \hat{a}^n \\ &= \sqrt{\frac{1!}{(1+n)!}} \hat{V}(1, 1) \hat{a}^n \\ &= \hat{P}(1, 1+n), \end{aligned} \tag{14.8}$$

$$\begin{aligned} \hat{P}(1, m)\hat{D} &= \hat{P}(1, 1+n) \hat{D} \\ &= \sqrt{\frac{1!}{(1+n)!}} \hat{P}(1, 1) \hat{a}^n \hat{D}. \end{aligned}$$

Then for

$$\hat{B} = \hat{A} \hat{a}^n \hat{D},$$

note that

$$\hat{A} = \sqrt{\frac{1!}{(1+n)!}} \hat{P}(1, 1),$$

$$[\hat{A}, \hat{a}^+ \hat{a}] = 0.$$

#### 14.4. Use of Generalized Bessel Functions

It is evident that different basis states, containing different boson factors, are effectively equivalent for various possible choices of  $\hat{A}$ . Among other things,  $\hat{A}$  could

be either a generalized Bessel function or unity. What this means in effect is that a generalized Bessel function can be inserted into or omitted from a basis state with impunity. In other words, it does not make any difference whether or not the generalized Bessel function is there. Because of the connection between the generalized Bessel function and the exponential displacement operator, it may be that the presence of the latter, even though it lacks time dependence, could negate in part the function of the former in a basis state. To the extent that this is true, any further inclusion of a generalized Bessel function would be unnecessary.

An exposition of a general solution for the Einstein model, providing an expression for the Green function, is available (Mahan 1981). An alternative approach to a solution, described in earlier chapters of the present dissertation, leads to expressions containing factors that can be written as generalized Bessel functions.

A Green function is generally expressible in the form

$$G_k(\vec{r}_1, \vec{r}_2) = \sum_{n=0}^{\infty} \frac{\phi_n(\vec{r}_1) \phi_n(\vec{r}_2)}{\lambda_n^k - \lambda^k},$$

where  $\vec{r}_1$  could be  $x$  and  $\vec{r}_2$  could be  $t$ . Thus the Green function involves sums of products of eigenfunctions (Arfken 1970). The eigenfunctions, in turn, can be composed of sums

of products of basis states representing elementary excitations of the system described by the Green function. Therefore, if the Green function does indeed involve generalized Bessel functions, it would seem then that some basis states should contain factors that are generalized Bessel functions. Such factors have boson stepping operators nicely arranged in normal ordering. It is largely because of this convenient ordering that the generalized Bessel functions seemed so attractive.

The conclusion that any such factors are extraneous is a puzzling and disappointing one, considering the initial promise shown by the generalized Bessel functions and the effort invested in their development. Indeed, they seem to arise so naturally in the search for solutions that it seems possible that they may yet prove to have some importance.

## 15. Projection-Operator Boson Factors

### 15.1. Projection-Operator Basis States

The simple relation

$$\begin{aligned}\langle 0 | \hat{a} \hat{a}^\dagger | 0 \rangle &= \langle 0 | (1 + \hat{a}^\dagger \hat{a}) | 0 \rangle \\ &= \langle 0 | 0 \rangle + \langle 0 | \hat{a}^\dagger \hat{a} | 0 \rangle = \langle 0 | 0 \rangle = 1 = 0!\end{aligned}$$

can be extended to show for example that

$$\langle 0 | \hat{a}^{n-1} (\hat{a}^\dagger)^{m-k} | 0 \rangle = \delta_{n-1, m-k} (n-1)!, \quad (15.1)$$

with the special case

$$\langle 0 | \hat{a}^m (\hat{a}^\dagger)^m | 0 \rangle = m!.$$

These relations will be used to calculate inner products.

Let the eigenfunction

$$\hat{\Psi}_n = \hat{c} \hat{a}^n \hat{D} = \sum_{m=0}^{\infty} \alpha(n, m) \hat{\Phi}_m = \sum_{m=0}^{\infty} \alpha_{nm} \hat{\Phi}_m \quad (15.2)$$

be composed of basis states

$$\hat{\Phi}_m = c | 0 \rangle \langle 0 | \hat{a}^m \quad (15.3)$$

where the zero states form a projection operator for bosons only.

Use Eq. (15.1) and Eq. (15.3) to form the inner product

$$\begin{aligned}((\hat{\Phi}_1, \hat{\Phi}_m)) &= \langle [\hat{\Phi}_m, \hat{\Phi}_1] \rangle \\ &= \langle \hat{\Phi}_m \hat{\Phi}_1^\dagger - \hat{\Phi}_1 \hat{\Phi}_m \rangle\end{aligned}$$

$$\begin{aligned}
&= \langle 0 | \hat{c} | 0 \rangle \langle 0 | \hat{a}^m (\hat{a}^+)^1 | 0 \rangle \\
&\quad \times \langle 0 | \hat{c}^+ - (\hat{a}^+)^1 | 0 \rangle \\
&\quad \times \langle 0 | \hat{c}^+ \hat{c} | 0 \rangle \langle 0 | \hat{a}^m | 0 \rangle \\
&= \delta_{m,1} \langle \hat{c} \hat{c}^+ \rangle \langle 0 | \hat{a}^m (\hat{a}^+)^1 | 0 \rangle. \tag{15.4}
\end{aligned}$$

From Eq. (15.2) and Eq. (15.3) form the inner product

$$\begin{aligned}
((\hat{\phi}_1, \hat{\psi}_n)) &= \langle [\hat{\psi}_n, \hat{\phi}_1^+] \rangle \\
&= \langle \hat{\psi}_n, \hat{\phi}_1^+ - \hat{\phi}_1^+ \hat{\psi}_n \rangle \\
&= \langle 0 | \hat{c} \hat{a}^n \hat{D} (\hat{a}^+)^1 | 0 \rangle \langle 0 | \hat{c}^+ - (\hat{a}^+)^1 | 0 \rangle \\
&\quad \times \langle 0 | \hat{c}^+ \hat{c} \hat{a}^n \hat{D} | 0 \rangle \\
&= \langle \hat{c} \hat{c}^+ \rangle \langle 0 | \hat{a}^n \hat{D} (\hat{a}^+)^1 | 0 \rangle. \tag{15.5}
\end{aligned}$$

From the relationship between the eigenfunctions and basis states it is possible to write

$$\begin{aligned}
((\hat{\phi}_1, \hat{\psi}_n)) &= \sum_{m=0}^{\infty} \alpha_{nm} ((\hat{\phi}_1, \hat{\phi}_m)) \\
&= \alpha_{n0} ((\hat{\phi}_1, \hat{\phi}_0)) + \dots \\
&\quad + \alpha_{n1} ((\hat{\phi}_1, \hat{\phi}_1)) + \dots \\
&= \alpha_{n1} ((\hat{\phi}_1, \hat{\phi}_1))
\end{aligned}$$

because

$$((\hat{\phi}_1, \hat{\phi}_n)) = \delta_{1n} ((\hat{\phi}_1, \hat{\phi}_n)).$$

Then

$$\alpha_{n1} = \frac{((\hat{\phi}_1, \hat{\psi}_n))}{((\hat{\phi}_1, \hat{\phi}_1))}$$

or

$$\alpha_{nm} = \frac{((\hat{\phi}_m, \hat{\psi}_n))}{((\hat{\phi}_m, \hat{\phi}_m))}. \quad (15.6)$$

Substituting the inner products from Eq. (15.4) and Eq. (15.5) into Eq. (15.6) gives

$$\begin{aligned} \alpha_{nm} &= \frac{\langle \hat{c}\hat{c}^+ \rangle \langle 0 | \hat{a}^{n\hat{D}} (\hat{a}^+)^m | 0 \rangle}{\langle \hat{c}\hat{c}^+ \rangle \langle 0 | \hat{a}^m (\hat{a}^+)^m | 0 \rangle} \\ &= \frac{\langle 0 | \hat{a}^{n\hat{D}} (\hat{a}^+)^m | 0 \rangle}{m!}. \end{aligned} \quad (15.7)$$

This must be evaluated.

## 15.2. Evaluation of Expectation Value

Using exponential expansions it is possible to show

$$[\hat{a}, e^{z\hat{a}^+}] = ze^{z\hat{a}^+}.$$

By generalizing

$$[\hat{a}\hat{a}, e^{z\hat{a}^+}] = \hat{a}[\hat{a}, e^{z\hat{a}^+}] + [\hat{a}, e^{z\hat{a}^+}]\hat{a}$$

it is further possible to show

$$[\hat{a}^n, e^{z\hat{a}^+}] = e^{z\hat{a}^+} [(z + \hat{a})^n - \hat{a}^n] \quad (15.8)$$

and

$$[e^{-z\hat{a}}, (\hat{a}^+)^n] = [(\hat{a}^+ - z)^n - (\hat{a}^+)^n]e^{-z\hat{a}}. \quad (15.9)$$

Use of the Campbell-Baker-Hausdorff theorem and

$$\langle 0 | \hat{a}^\dagger = 0,$$

$$\hat{a} | 0 \rangle = 0,$$

along with the commutators given by Eq. (15.8) and Eq. (15.9), makes it possible to work towards evaluating Eq. (15.7) by writing

$$\begin{aligned} L(n, m) &\equiv e^{z^2/2} \langle 0 | \hat{a}^n \hat{D}(\hat{a}^\dagger)^m | 0 \rangle \\ &= \langle 0 | [\hat{a}^n, e^{z\hat{a}^\dagger}] [e^{-z\hat{a}}, (\hat{a}^\dagger)^m] | 0 \rangle \\ &= \langle 0 | e^{z\hat{a}^\dagger} [(a + \hat{a})^n - \hat{a}^n] \\ &\quad \times [(\hat{a}^\dagger - z)^m - (\hat{a}^\dagger)^m] e^{-z\hat{a}} | 0 \rangle \\ &= \sum_{l=0}^{\infty} \sum_{k=0}^{\infty} \frac{n!m!(-z)^k z^l \delta_{n-1, m-k}}{l!(n-1)!k!(m-k)!} \\ &\quad \times (n-1)! \end{aligned}$$

Using  $k = m - n + 1$  get

$$\begin{aligned} L(n, m) &= \sum_{l=0}^n \sum_{l+m-n=0}^{l+m-n=m} \frac{n!m!(-z)^{l+m-n} z^l (n-1)!}{l!(n-1)!(l+m-n)!} \\ &\quad \times \frac{1}{(n-1)!} \\ &= \sum_{l=0}^n \frac{(n!)^2 (-1)^l z^{2l}}{(l!)^2 n!}, \quad n = m. \end{aligned} \quad (15.10)$$

### 15.3. Associated Laguerre Polynomials

The associated Laguerre polynomials are (Arfken 1970)

$$L_n^k(x) = \sum_{m=0}^n \frac{(-1)^m (n+k)! x^m}{(n-m)! (k+m)! m!}, \quad k > -1. \quad (15.11)$$

With the help of Eq. (15.11) it is possible to rewrite Eq. (15.10)

$$\begin{aligned} L(n, m) &= n! (-z)^{m-n} L_m^{m-n}(z^2), \quad m \geq n \\ &= m! z^{n-m} L_m^{n-m}(z^2), \quad n \geq m \\ &= n! L_n^0(z^2), \quad n=m, \end{aligned}$$

and so it is finally possible to evaluate

$$\begin{aligned} \alpha(n, m) &= e^{-z^2/2} \frac{n!}{m!} (-z)^{m-n} L_n^{m-n}(z^2), \quad m \geq n \\ &= e^{-z^2/2} z^{m-n} L_n^{m-n}(z^2), \quad n \geq m \\ &= e^{-z^2/2} L_n^0(z^2), \quad n=m. \end{aligned}$$

For  $n = m$  get

$$\begin{aligned} n! L_n^0(z^2) &= e^{-z^2/2} n! \alpha(n, m) \\ &= e^{-z^2/2} \langle 0 | \frac{\hat{a}^n}{\sqrt{n!}} \hat{D}(\hat{a}^+) | 0 \rangle. \end{aligned}$$

This matches (Mahan 1981:276)

$$n! L_n^0(z^2) = \langle n | e^{z\hat{a}^+} e^{-z\hat{a}} | n \rangle$$

$$\begin{aligned} &= e^{-z^2/2} \langle n | \hat{D} | n \rangle \\ &= e^{-z^2/2} \langle 0 | \frac{\hat{a}^n \hat{D} (\hat{a}^\dagger)^n}{\sqrt{n!} \sqrt{n!}} | 0 \rangle. \end{aligned}$$

## 16. Einstein and Simplified Dirac Models

### 16.1. Simple Solution of Einstein Model

The deceptive appearance of the stripped-down Hamiltonian operators that are employed as approximate models of simple many-particle systems in condensed-matter physics has been pointed out in a recent reference (Mahan 1981:24). "Usually these Hamiltonians look very simple but still are impossible to solve exactly. Often they are even difficult to solve approximately!" The Hamiltonian operators describing systems with fermion-boson interactions can be especially difficult to solve. As it happens, eigenvalues of the Hamiltonian operator for the Einstein model can be found in a simple and direct way.

The Hamiltonian operator for the Einstein model is

$$\hat{H} = \omega_0 \hat{a}^\dagger \hat{a} + \omega_0 \lambda_0 \hat{c}^\dagger \hat{c} (\hat{a} + \hat{a}^\dagger) + \epsilon_c \hat{c}^\dagger \hat{c}.$$

Assume a basis state that is a product of a fermion factor and a boson factor:

$$\hat{\phi} = \hat{F}\hat{B}.$$

Calculate

$$\begin{aligned} \hat{L}\hat{\phi} &= [\hat{\phi}, \hat{H}] \\ &= \omega_0 [\hat{F}\hat{B}, \hat{a}^\dagger \hat{a}] + \omega_0 \lambda_0 [\hat{F}\hat{B}, \hat{c}^\dagger \hat{c} (\hat{a} + \hat{a}^\dagger)] \end{aligned}$$

$$\begin{aligned}
& + \epsilon_c [\hat{F}\hat{B}, \hat{c}^+\hat{c}] \\
& = \omega_o \hat{F} [\hat{B}, \hat{a}^+\hat{a}] + \omega_o \lambda_o \hat{F} \hat{c}^+ \hat{c} \hat{B} (\hat{a} + \hat{a}^+) \\
& \quad - \omega_o \lambda_o \hat{c}^+ \hat{c} \hat{F} (\hat{a} + \hat{a}^+) \hat{B} + \epsilon_c [\hat{F}, \hat{c}^+ \hat{c}] \hat{B}.
\end{aligned}$$

For

$$\hat{F} = \hat{c}$$

get

$$\hat{F} \hat{c}^+ \hat{c} = \hat{F},$$

$$\hat{c}^+ \hat{c} \hat{F} = 0,$$

$$\hat{L}\hat{\phi} = \hat{F}\omega_o [\hat{B}, \hat{a}^+\hat{a}] + \hat{F}\omega_o \lambda_o \hat{B} (\hat{a} + \hat{a}^+) + \epsilon_c \hat{F}\hat{B}.$$

For

$$\hat{B} = \hat{A} \hat{a}^n \hat{D}$$

substitute from Eq. (14.5) to get

$$\hat{L}\hat{\phi} = (\epsilon_c + n\omega_o - \lambda_o^2 \omega_o) \hat{\phi} + \hat{F}\omega_o [\hat{A}, \hat{a}^+\hat{a}] \hat{a}^n \hat{D}.$$

For

$$[\hat{A}, \hat{a}^+\hat{a}] = 0,$$

the basis state is an eigenfunction.

The eigenvalues just obtained for the Einstein model resemble those for the displaced harmonic oscillator, except that the solution for the Einstein model contains an additional term arising from the presence, in the Hamiltonian operator for this model, of an extra term

containing the fermion number operator.

A displacement term that is linear in the coupling coefficient appears in the Hamiltonian operators for both the Einstein model and the displaced harmonic oscillator. The sign of this term is positive for the Einstein model and negative for the displaced harmonic oscillator. An eigenvalue for either of these two models contains a term that is quadratic rather than linear in the coupling coefficient. The sign of this term is positive for each of the two models. Changing the sign of the coupling coefficient in the Hamiltonian operator does not change the sign of the quadratic term in the eigenvalue.

## 16.2. Projection-Operator Solution

Using the basis state

$$\hat{\phi}_m = \hat{c} |0\rangle \langle 0| \hat{a}^{mD}$$

with the Einstein Hamiltonian operator

$$\hat{H} = \omega_0 \hat{a}^\dagger \hat{a} + \omega_0 \lambda_0 \hat{c}^\dagger \hat{c} (\hat{a} + \hat{a}^\dagger) + \epsilon_c \hat{c}^\dagger \hat{c}$$

gives

$$\begin{aligned} \hat{L} \hat{\phi}_m &= \epsilon_c \hat{\phi}_m + m \omega_0 \hat{\phi}_m \\ &= \omega_0 \lambda_0 \hat{c} |0\rangle \langle 0| \hat{a}^m (\hat{a} + \hat{a}^\dagger) \\ &= \epsilon_c \hat{\phi}_m + n \omega_0 \hat{\phi}_m + \omega_0 \lambda_0 \hat{\phi}_{m+1} + \omega_0 \lambda_0 m \hat{\phi}_{m-1}. \end{aligned}$$

It has already been shown that

$$\hat{\Psi}_n = \hat{c} \hat{a}^n \hat{D}$$

is an eigenvector of the Einstein Hamiltonian operator, with eigenvalue

$$\epsilon = \epsilon_c + n\omega_0 - \lambda_0^2 \omega_0.$$

If the eigenvector is composed of basis states through the relation

$$\hat{\Psi}_n = \sum_{m=0}^{\infty} \alpha_{nm} \hat{\phi}_m,$$

it is possible to write

$$\hat{L} \hat{\Psi}_n = (\epsilon_c + n\omega_0 - \lambda_0^2 \omega_0) \hat{\Psi}_n$$

$$= \sum_{m=0}^{\infty} \alpha_{nm} \hat{L} \hat{\phi}_m,$$

$$\begin{aligned} (\hat{L} - \epsilon_c) \hat{\Psi}_n &= \sum_{m=0}^{\infty} \alpha_{nm} m \omega_0 \hat{\phi}_m + \sum_{m=0}^{\infty} \alpha_{nm} \omega_0 \lambda_0 \hat{\phi}_{m+1} \\ &\quad + \sum_{m=0}^{\infty} m \alpha_{nm} \omega_0 \lambda_0 \hat{\phi}_{m-1}. \end{aligned}$$

In the first and third sums, there is no term for zero  $m$ .

It is useful to substitute

$$m = m' - 1$$

in the second sum and

$$m = m' + 1$$

in the third sum. These substitutions give

$$\begin{aligned}
(\hat{L} - \epsilon_c) \hat{\Psi}_n &= \omega_0 \sum_{m=0}^{\infty} \alpha_{nm} m \hat{\Phi}_m \\
&+ \omega_0 \lambda_0 \sum_{m'=1}^{\infty} \alpha_{n(m'-1)} \hat{\Phi}_{m'} \\
&+ \omega_0 \lambda_0 \sum_{m'=0}^{\infty} (m'+1) \alpha_{n(m'+1)} \hat{\Phi}_{m'} \\
&= \omega_0 \sum_{m=0}^{\infty} [m \alpha_{nm} + \lambda_0 \alpha_{n(m-1)} \\
&+ \lambda_0 (m+1) \alpha_{n(m+1)}] \hat{\Phi}_m.
\end{aligned}$$

This should equal

$$\begin{aligned}
(\hat{L} - \epsilon_c) \hat{\Psi}_n &= \omega_0 (n - \lambda_0^2) \hat{\Psi}_n \\
&= \omega_0 \sum_{m=0}^{\infty} \alpha_{nm} (n - \lambda_0^2) \hat{\Phi}_m.
\end{aligned}$$

This can happen only if the following balancing equation holds:

$$\begin{aligned}
(m - n + \lambda_0^2) \alpha(n, m) + \lambda_0 \alpha(n, m-1) \\
+ \lambda_0 (m+1) \alpha(n, m+1) = 0 \quad \forall n, m.
\end{aligned}$$

Check this for  $m \geq n$  by setting  $z = \lambda_0$  in Eq. (16.14) to get

$$\alpha(n, m) = \sum_{l=0}^n \frac{n! (-1)^{l+m-n} \lambda_0^{2l+m-n}}{l! (1+m-n)! (n-l)!},$$

$$\alpha(n, m-1) = \sum_{l=0}^n \frac{n!(-1)^{l+m-n-1} z^{2l+m-n}}{l!(l+m-1-n)!(n-l)!},$$

$$\alpha(n, m+1) = \sum_{l=0}^n \frac{n!(-1)^{l+m-n+1} z^{2l+m-n+1}}{l!(l+m+1-n)!(n-l)!},$$

and by substituting these coefficients into the balancing equation to show

$$\sum_{l=0}^n \frac{n!(-1)^{l+m-n} z^{2l+m-n}}{l!(n-l)!(l+m-n)!} \left[ -1 - \frac{z^2(n-l)}{l+m+1-n} \right] = 0.$$

### 16.3. Solution of Simplified Dirac Model

The Hamiltonian operator for the Dirac model is

$$\hat{H} = \omega_0 \hat{a}^\dagger \hat{a} + \omega_0 \lambda_0 (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) (\hat{a} + \hat{a}^\dagger) + \epsilon_c \hat{c}^\dagger \hat{c} + \epsilon_b \hat{b}^\dagger \hat{b}.$$

Assume a basis state that is a product of a fermion factor and a boson factor:

$$\hat{\phi} = \hat{F}\hat{B}.$$

Calculate

$$\begin{aligned} \hat{L}\hat{\phi} &= [\hat{\phi}, \hat{H}] \\ &= \omega_0 [\hat{F}\hat{B}, \hat{a}^\dagger \hat{a}] + \omega_0 \lambda_0 [\hat{F}\hat{B}, (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) (\hat{a} + \hat{a}^\dagger)] \\ &\quad + \epsilon_c [\hat{F}\hat{B}, \hat{c}^\dagger \hat{c}] + \epsilon_b [\hat{F}\hat{B}, \hat{b}^\dagger \hat{b}]. \end{aligned}$$

Consider two different fermion operators,

$$\hat{F}_b = \hat{c}\hat{c}^\dagger\hat{b},$$

$$\hat{F}_c = \hat{b}\hat{b}^\dagger\hat{c},$$

which can be added and subtracted to form a pair of fermion factors:

$$\hat{F}_p = \hat{F}_b + \hat{F}_c,$$

$$\hat{F}_m = \hat{F}_b - \hat{F}_c.$$

For

$$\hat{F} = \hat{F}_p$$

get

$$\hat{F}_p(\hat{c}^\dagger\hat{b} + \hat{b}^\dagger\hat{c}) = \hat{F}_p,$$

$$(\hat{c}^\dagger\hat{b} + \hat{b}^\dagger\hat{c})\hat{F}_p = 0,$$

$$[\hat{F}_p, \epsilon_b\hat{b}^\dagger\hat{b} + \epsilon_c\hat{c}^\dagger\hat{c}] = \epsilon_b\hat{c}\hat{c}^\dagger\hat{b} + \epsilon_c\hat{b}\hat{b}^\dagger\hat{c}.$$

For

$$\hat{\phi} = \hat{\phi}_p = \hat{F}_p\hat{B} = \hat{F}_p\hat{B}_p$$

get

$$\begin{aligned} \hat{L}\hat{\phi}_p &= [\hat{\phi}_p, \hat{H}] \\ &= \hat{F}_p\omega_0[\hat{B}_p, \hat{a}^\dagger\hat{a}] + \hat{F}_p\omega_0\lambda_0\hat{B}_p(\hat{a} + \hat{a}^\dagger) \\ &\quad + \epsilon_c\hat{b}\hat{b}^\dagger\hat{c}\hat{B}_p + \epsilon_b\hat{c}\hat{c}^\dagger\hat{b}\hat{B}_p. \end{aligned}$$

Then for

$$\hat{B} = \hat{B}_p = \hat{A} \hat{a} \hat{n} \hat{D}$$

get

$$\begin{aligned} \hat{L} \hat{\Phi}_p &= (n\omega_0 - \lambda_0^2 \omega_0) \hat{\Phi}_p + \hat{F}_p \omega_0 [\hat{A}, \hat{a}^\dagger \hat{a}] \hat{a} \hat{n} \hat{D} \\ &+ \epsilon_c \hat{b} \hat{b}^\dagger \hat{c} \hat{B}_p + \epsilon_b \hat{c} \hat{c}^\dagger \hat{b} \hat{B}_p. \end{aligned}$$

A single eigenvector does not span a space; there exists a normal eigenvector also.

From two orthogonal fermion basis states

$$\hat{x} = \hat{c},$$

$$\hat{y} = \hat{b},$$

it is possible to construct the fermion parts of an orthogonal pair of eigenvectors in the forms

$$\hat{F}_p = \frac{1}{\sqrt{2}} (\hat{x} + \hat{y}),$$

$$\hat{F}_n = \frac{1}{\sqrt{2}} (\hat{x} - \hat{y}).$$

From two basis states

$$\hat{x} = \hat{b} \hat{b}^\dagger \hat{c}$$

$$\hat{y} = \hat{c} \hat{c}^\dagger \hat{b},$$

it is possible to construct the fermion part

$$\hat{F}_p = \hat{b} \hat{b}^\dagger \hat{c} + \hat{c} \hat{c}^\dagger \hat{b}$$

of an eigenvector. Because of the nonorthogonality of the two basis states in this sum, the fermion part of the normal

eigenvector is not simply the difference

$$\hat{F}_m = \hat{b}\hat{b}^+\hat{c} - \hat{c}\hat{c}^+\hat{b},$$

unless the two eigenvectors differ in some other way as well.

For

$$\hat{F} = \hat{F}_m$$

get

$$\hat{F}_m(\hat{c}^+\hat{b} + \hat{b}^+\hat{c}) = 0,$$

$$(\hat{c}^+\hat{b} + \hat{b}^+\hat{c})\hat{F}_m = -\hat{F}_m,$$

$$[\hat{F}_m, \epsilon_c \hat{c}^+\hat{c} + \epsilon_b \hat{b}^+\hat{b}] = \epsilon_c \hat{c}^+\hat{c}\hat{b} - \epsilon_b \hat{b}^+\hat{b}\hat{c}.$$

For

$$\hat{\phi} = \hat{\phi}_m = \hat{F}_m \hat{B}_m$$

get

$$\hat{L}\hat{\phi}_m = [\hat{\phi}_m, \hat{H}]$$

$$= \hat{F}_m \omega_0 [\hat{B}_m, \hat{a}^+\hat{a}] + \hat{F}_m \omega_0 \lambda_0 (\hat{a} + \hat{a}^+) \hat{B}_m$$

$$+ \epsilon_c \hat{c}^+\hat{c} \hat{b} \hat{B}_m - \epsilon_b \hat{b}^+\hat{b} \hat{c} \hat{B}_m.$$

Then for

$$\hat{B}_m = \hat{D} \hat{a}^n \hat{A}$$

get

$$\begin{aligned} \hat{L}\hat{\Phi}_m &= (n\omega_0 + \lambda_0^2\omega_0)\hat{\Phi}_m + \hat{F}_m\omega_0\hat{D}a^n[\hat{A}, \hat{a}^+\hat{a}] \\ &+ \epsilon_c\hat{c}^+\hat{c}\hat{b}\hat{B}_m - \epsilon_b\hat{b}^+\hat{b}\hat{c}\hat{B}_m. \end{aligned}$$

As has been demonstrated previously, it is possible to construct an  $\hat{A}$  such that

$$[\hat{A}, \hat{a}^+\hat{a}] = 0.$$

For the special case

$$\epsilon_b = \epsilon_c = \epsilon_0,$$

the Dirac model has much the same basic symmetry as the Einstein model, and has the two independent solutions

$$\hat{L}\hat{\Psi}_p = (\epsilon_0 + n\omega_0 - \lambda_0^2\omega_0)\hat{\Psi}_p,$$

$$\hat{L}\hat{\Psi}_m = (\epsilon_0 + n\omega_0 + \lambda_0^2\omega_0)\hat{\Psi}_m,$$

with corresponding eigenvectors

$$\hat{\Psi}_p = (\hat{c}\hat{c}^+\hat{b} + \hat{b}\hat{b}^+\hat{c})\hat{A}a^n\hat{D},$$

$$\hat{\Psi}_m = (\hat{c}\hat{c}^+\hat{b} - \hat{b}\hat{b}^+\hat{c})\hat{D}a^n\hat{A}.$$

For other than this special case, a matrix solution, like the one to be described for the Lee model, is required.

## 17. Lee Model

### 17.1. Factorization of Basis State

The Hamiltonian operator for the Lee model is

$$\hat{H} = \omega_0 \hat{a}^\dagger \hat{a} + \lambda_0 \omega_0 \hat{c}^\dagger \hat{b} \hat{a}^\dagger + \lambda_0 \omega_0 \hat{b}^\dagger \hat{c} \hat{a} + \epsilon_b \hat{b}^\dagger \hat{b} + \epsilon_c \hat{c}^\dagger \hat{c}.$$

Let a basis state be a product of a fermion factor  $\hat{F}$  and a boson factor  $\hat{B}$ :

$$\hat{\phi} = \hat{F} \hat{B}.$$

Calculate

$$\begin{aligned} \hat{L} \hat{\phi} &= [\hat{\phi}, \hat{H}] \\ &= \omega_0 [\hat{F} \hat{B}, \hat{a}^\dagger \hat{a}] + \lambda_0 \omega_0 [\hat{F} \hat{B}, \hat{c}^\dagger \hat{b} \hat{a}^\dagger + \hat{b}^\dagger \hat{c} \hat{a}] \\ &\quad + \epsilon_b [\hat{F} \hat{B}, \hat{b}^\dagger \hat{b}] + \epsilon_c [\hat{F} \hat{B}, \hat{c}^\dagger \hat{c}] \\ &= \omega_0 \hat{F} [\hat{B}, \hat{a}^\dagger \hat{a}] \\ &\quad + \lambda_0 \omega_0 \hat{F} \hat{c}^\dagger \hat{b} \hat{B} \hat{a}^\dagger - \lambda_0 \omega_0 \hat{c}^\dagger \hat{b} \hat{F} \hat{a}^\dagger \hat{B} \\ &\quad + \lambda_0 \omega_0 \hat{F} \hat{b}^\dagger \hat{c} \hat{B} \hat{a} - \lambda_0 \omega_0 \hat{b}^\dagger \hat{c} \hat{F} \hat{a} \hat{B} \\ &\quad + \epsilon_b \hat{B} \hat{F} \hat{b}^\dagger \hat{b} + \epsilon_c \hat{B} \hat{F} \hat{c}^\dagger \hat{c} \\ &\quad - \epsilon_b \hat{B} \hat{b}^\dagger \hat{b} \hat{F} - \epsilon_c \hat{B} \hat{c}^\dagger \hat{c} \hat{F}. \end{aligned}$$

### 17.2. Fermion Factor

Some of the symmetry inherent in the Einstein model is lost in the Lee model because of the absence of certain

terms in the Hamiltonian operator for the Lee model. A method of solution for the Lee model must differ from any used for the Einstein model by addressing the asymmetry in the Lee model. The eigenfunctions for the Einstein model do not satisfy the Lee model; a cancellation of terms that occurs for the Einstein model does not occur for the Lee model because of the absent terms.

The hint as to how to construct a solution for the Lee model is inspired by Dirac's matrix solution for a relativistic Schroedinger equation (Saxon 1968). The first step towards a solution of the Lee model is the use of not one but two different fermion factors:

$$\hat{F}_b = \hat{c}\hat{c}^+\hat{b},$$

$$\hat{F}_c = \hat{b}\hat{b}^+\hat{c}.$$

For

$$\hat{F} = \hat{F}_b$$

get

$$\hat{F}\hat{b}^+\hat{c} = \hat{F}_c,$$

$$\hat{F}\hat{c}^+\hat{b} = \hat{c}^+\hat{b}\hat{F} = \hat{b}^+\hat{c}\hat{F} = 0,$$

$$\hat{F}\hat{b}^+\hat{b} = \hat{F}_b,$$

$$\hat{F}\hat{c}^+\hat{c} = \hat{b}^+\hat{b}\hat{F} = \hat{c}^+\hat{c}\hat{F} = 0.$$

For

$$\hat{F} = \hat{F}_c$$

get

$$\hat{F}\hat{c}^+\hat{b} = \hat{c}^+\hat{b}\hat{F} = \hat{b}^+\hat{c}\hat{F} = 0,$$

$$\hat{F}\hat{b}^+\hat{c} = \hat{F}_c,$$

$$\hat{F}\hat{b}^+\hat{b} = \hat{b}^+\hat{b}\hat{F} = \hat{c}^+\hat{c}\hat{F} = 0,$$

$$\hat{F}\hat{c}^+\hat{c} = \hat{F}_c.$$

For

$$\hat{\phi} = \hat{\phi}_b = \hat{F}_b \hat{B}$$

get

$$\hat{L}\hat{\phi}_b = \hat{F}_b \omega_0 [\hat{B}, \hat{a}^+\hat{a}] + \omega_0 \lambda_0 \hat{F}_c \hat{B} \hat{a} + \epsilon_b \hat{B} \hat{F}_b.$$

For

$$\hat{\phi} = \hat{\phi}_c = \hat{F}_c \hat{B}$$

get

$$\hat{L}\hat{\phi}_c = \hat{F}_c \omega_0 [\hat{B}, \hat{a}^+\hat{a}] + \omega_0 \lambda_0 \hat{F}_b \hat{B} \hat{a} + \epsilon_b \hat{B} \hat{F}_b.$$

### 17.3. Boson Factor

For

$$\hat{B} = \hat{P}(m, n) = \hat{P}(m, 0) \hat{a}^n$$

get

$$\hat{\phi}_b = \hat{\phi}_b(m, n) = \hat{F}_b \hat{P}(m, n),$$

$$\hat{\phi}_c = \hat{\phi}_c(m, n) = \hat{F}_c \hat{P}(m, n),$$

and

$$\begin{aligned} \hat{L}\hat{\phi}_b(m, n) &= \hat{F}_b \omega_o [\hat{P}(m, n), \hat{a}^+ \hat{a}] \\ &+ \omega_o \lambda_o \hat{F}_c \hat{P}(m, n) \hat{a} \\ &+ \epsilon_b \hat{P}(m, n) \hat{F}_b, \end{aligned}$$

$$\begin{aligned} \hat{L}\hat{\phi}_c(m, n) &= \hat{F}_c \omega_o [\hat{P}(m, n), \hat{a}^+ \hat{a}] \\ &+ \omega_o \lambda_o \hat{F}_c \hat{P}(m, n) \hat{a}^+ \\ &+ \epsilon_c \hat{P}(m, n) \hat{F}_c. \end{aligned}$$

Using Eq.(14.7) and Eq. (14.8), these last equations can be rewritten as

$$\begin{aligned} \hat{L}\hat{\phi}_b(m, n) &= (n - m) \omega_o \hat{F}_b \hat{P}(m, n) \\ &+ \sqrt{n + 1} \omega_o \lambda_o \hat{F}_c \hat{P}(m, n + 1) \\ &+ \epsilon_b \hat{F}_b \hat{P}(m, n), \end{aligned}$$

$$\begin{aligned} \hat{L}\hat{\phi}_c(m, n) &= (n - m) \omega_o \hat{F}_c \hat{P}(m, n) \\ &+ \sqrt{n} \omega_o \lambda_o \hat{F}_b \hat{P}(m, n - 1) \\ &+ \epsilon_c \hat{F}_c \hat{P}(m, n). \end{aligned}$$

By substituting  $n + 1$  for  $n$ , the second equation can be altered to

$$\begin{aligned} \hat{L}\hat{\Phi}_c(m, n+1) &= (n-m+1)\omega \hat{F}_o \hat{P}_c(m, n+1) \\ &+ \sqrt{n+1} \omega_o \lambda_o \hat{F}_b \hat{P}(m, n) \\ &+ \epsilon_c \hat{F}_c \hat{P}(m, n+1). \end{aligned}$$

#### 17.4. Matrix Solutions

Both equations can be combined into a single matrix equation:

$$\begin{aligned} \hat{L} \begin{bmatrix} \hat{\Phi}_b(m, n) \\ \hat{\Phi}_c(m, n+1) \end{bmatrix} &= \begin{bmatrix} (n-m)\omega_o + \epsilon_b & \omega_o \lambda_o \sqrt{n+1} \\ \omega_o \lambda_o \sqrt{n+1} & (n-m+1)\omega_o + \epsilon_c \end{bmatrix} \\ &\times \begin{bmatrix} \hat{\Phi}_b(m, n) \\ \hat{\Phi}_c(m, n+1) \end{bmatrix}, \end{aligned}$$

or

$$\hat{L}\hat{\Phi} = \hat{A}\hat{\Phi},$$

where

$$\hat{\Phi} = \begin{bmatrix} \hat{\Phi}_b(m, n) \\ \hat{\Phi}_c(m, n+1) \end{bmatrix},$$

$$\tilde{A} = \begin{bmatrix} (n - m)\omega_0 + \epsilon_b & \omega_0 \lambda_0 \sqrt{n + 1} \\ \omega_0 \lambda_0 \sqrt{n + 1} & (n - m + 1)\omega_0 + \epsilon_c \end{bmatrix}.$$

The eigenvalues and eigenvectors of  $\hat{L}$  can be found by diagonalizing  $\tilde{A}$ . Let  $\tilde{A}$  be diagonalized by a similarity transformation

$$\tilde{X}^+ \tilde{A} \tilde{X} = \tilde{\lambda},$$

where  $\tilde{\lambda}$  is a matrix of eigenvalues. Then

$$\tilde{A} \hat{\phi} = \tilde{X} \tilde{\lambda} \tilde{X}^+ \hat{\phi},$$

$$\Rightarrow \tilde{X}^+ \tilde{A} \hat{\phi} = \tilde{\lambda} \tilde{X}^+ \hat{\phi},$$

$$\Rightarrow \tilde{X}^+ \tilde{A} \tilde{X} \tilde{X}^+ \hat{\phi} = \tilde{\lambda} \tilde{X}^+ \hat{\phi},$$

$$\Rightarrow \tilde{X}^+ \tilde{A} \tilde{X} \hat{\psi} = \tilde{\lambda} \hat{\psi},$$

where the eigenvectors of  $\hat{L}$  are (Symon 1971:415-424)

$$\tilde{\psi} = \tilde{X}^+ \hat{\phi}.$$

### 17.5. Eigenvalue Problem

The matrix equation

$$(\tilde{A} - \tilde{\lambda}) \tilde{X} = 0$$

is here equivalent to a pair of simultaneous equations:

$$(a_{11} - \lambda_i) X_{1i} + a_{12} X_{2i} = 0,$$

$$a_{21} X_{1i} + (a_{22} - \lambda_i) X_{2i} = 0.$$

A trivial solution is

$$X_{2i} = 0.$$

The other solution,

$$(a_{11} - \lambda_1)(a_{22} - \lambda_1) - a_{21}a_{12} = 0,$$

is the secular or characteristic equation

$$\lambda_1^2 - \lambda_1(a_{11} + a_{22}) + a_{11}a_{22} - a_{21}a_{12} = 0.$$

The roots of the secular equation are the two eigenvalues

$$\lambda_{1,2} = \frac{a_{11} + a_{22}}{2} \pm \sqrt{\left[\frac{a_{11} + a_{22}}{2}\right]^2 - (a_{11}a_{22} - a_{21}a_{12})}.$$

Substitution of an eigenvalue back into the simultaneous equations gives

$$x_{2i} = - \frac{(a_{11} - \lambda_i)}{a_{12}} x_{1i}.$$

Substitution of this relation into the normalization condition

$$x_{1i}^2 + x_{2i}^2 = 1$$

gives one component of an eigenvector of the A matrix,

$$x_{1i} = \frac{1}{\sqrt{1 + \left[\frac{a_{11} - \lambda_i}{a_{12}}\right]^2}}.$$

The second component of the eigenvector can be found by substituting the first component back into one of the simultaneous equations. The components of the second eigenvector can be found from the other eigenvalue.

The method of solution for the eigenvalues indicates that the X matrix should be unitary. Then an eigenvector of the Liouville superoperator can be found from

$$\begin{bmatrix} \hat{\Psi}_b(m, n) \\ \hat{\Psi}_c(m, n+1) \end{bmatrix} = \begin{bmatrix} X_{11} & X_{21} \\ X_{12} & X_{22} \end{bmatrix} \begin{bmatrix} \hat{\Phi}_b(m, n) \\ \hat{\Phi}_c(m, n+1) \end{bmatrix}.$$

### 17.6. Eigenvalues for Lee Model

The eigenvalues for the Lee model are found to be

$$\begin{aligned} \lambda_{1,2} = & \frac{\epsilon_b + \epsilon_c + [2(n-m) + 1]\omega_0}{2} \\ & \pm \left[ \left[ \frac{\epsilon_b - \epsilon_c + \omega_0}{2} \right]^2 + [(n-m) + 1] \right. \\ & \left. \times (\omega_0 \lambda_0)^2 \right]^{1/2}. \end{aligned}$$

For

$$\epsilon_b = \epsilon_c = 0,$$

the eigenvalues reduce to

$$\begin{aligned} \lambda_{1,2} = & [2(n-m) + 1] \frac{\omega_0}{2} \pm \left[ \left[ \frac{\omega_0}{2} \right]^2 \right. \\ & \left. + [(n-m) + 1] (\omega_0 \lambda_0)^2 \right]^{1/2}. \end{aligned}$$

The restriction

$$\lambda_0 = 0$$

diagonalizes the A matrix, immediately yielding the eigenvalues

$$\lambda_1 = (n - m + 1)\omega_0 + \epsilon_c,$$

$$\lambda_2 = (n - m)\omega_0 + \epsilon_b.$$

The corresponding eigenvectors of the Liouville superoperator are then simply

$$\begin{aligned}\hat{\Psi}_1 &= \hat{\Phi}_c(m, n + 1) \\ &= \hat{b}\hat{b}^+\hat{c}\hat{P}(m, n + 1),\end{aligned}$$

$$\begin{aligned}\hat{\Psi}_2 &= \hat{\Phi}_b(m, n) \\ &= \hat{c}\hat{c}^+\hat{b}\hat{P}(m, n).\end{aligned}$$

## 18. Dirac Model

### 18.1. Basis State

For

$$\hat{\phi} = \hat{F} \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m,$$

calculate

$$\begin{aligned} \hat{L}\hat{\phi} &= [\hat{\phi}, \hat{H}] \\ &= [\hat{F}, \epsilon_b \hat{b}^\dagger \hat{b} + \epsilon_c \hat{c}^\dagger \hat{c}] \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m \\ &\quad + \lambda_0 \omega_0 \hat{F} (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) \\ &\quad \times \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m (\hat{a}^\dagger + \hat{a}) \\ &\quad - \lambda_0 \omega_0 (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) \hat{F} \\ &\quad \times \sum_{m=0}^{\infty} \alpha(n, m) (\hat{a}^\dagger + \hat{a}) |0\rangle \langle 0| \hat{a}^m \\ &\quad + \omega_0 \hat{F} \left[ \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m, \hat{a}^\dagger \hat{a} \right]. \end{aligned}$$

### 18.2. Calculation of Boson Factors

Evaluate

$$\left[ \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m, \hat{a}^\dagger \hat{a} \right]$$

$$\begin{aligned}
&= \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m \hat{a}^\dagger \hat{a} \\
&\quad - \sum_{m=0}^{\infty} \alpha(n, m) \hat{a}^\dagger \hat{a} |0\rangle \langle 0| \hat{a}^m \\
&= \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| (m \hat{a}^{m-1} + \hat{a}^\dagger \hat{a}^m) \hat{a} \\
&= \sum_{m=0}^{\infty} m \alpha(n, m) |0\rangle \langle 0| \hat{a}^m.
\end{aligned}$$

Evaluate

$$\begin{aligned}
&\sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m (\hat{a}^\dagger + \hat{a}) \\
&= \sum_{m=0}^{\infty} (m+1) \alpha(n, m+1) |0\rangle \langle 0| \hat{a}^m \\
&\quad + \sum_{m=0}^{\infty} \alpha(n, m-1) |0\rangle \langle 0| \hat{a}^m.
\end{aligned}$$

In the first term on the right-hand side, the factor  $(m+1)$  causes the vanishing of the term for  $m+1=0$ . In the second term on the right-hand side, the terms  $[1+(m-n)]!$  and  $m!$  in the denominator of  $\alpha(n, m-1)$  causes the vanishing of the term for  $m-1=0$ .

Substitute the evaluated terms to get

$$\begin{aligned}
\hat{L}\hat{\Phi} &= [\hat{F}, \epsilon_b \hat{b}^\dagger \hat{b} + \epsilon_c \hat{c}^\dagger \hat{c}] \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle \langle 0| \hat{a}^m \\
&\quad + \lambda_o \omega_o \hat{F} (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c})
\end{aligned}$$

$$\begin{aligned}
& \times \sum_{m=0}^{\infty} (m+1) \alpha(n, m+1) |0\rangle \langle 0| \hat{a}^m \\
& + \lambda_0 \omega_0 \hat{F} (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) \\
& \times \sum_{m=0}^{\infty} \alpha(n, m-1) |0\rangle \langle 0| \hat{a}^m \\
& - \lambda_0 \omega_0 (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) \hat{F} \\
& \times \sum_{m=0}^{\infty} \alpha(n, m) (\hat{a}^\dagger + \hat{a}) |0\rangle \langle 0| \hat{a}^m \\
& + \omega_0 \hat{F} \sum_{m=0}^{\infty} m \alpha(n, m) (\hat{a}^\dagger)^m |0\rangle \langle 0|.
\end{aligned}$$

### 18.3. Fermion Factors

For

$$\hat{F} = \hat{b} \hat{b}^\dagger \hat{c},$$

get

$$[\hat{b} \hat{b}^\dagger \hat{c}, \epsilon_b \hat{b}^\dagger \hat{b} + \epsilon_c \hat{c}^\dagger \hat{c}] = \epsilon_c \hat{b} \hat{b}^\dagger \hat{c},$$

$$\hat{b} \hat{b}^\dagger \hat{c} (\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) = \hat{c} \hat{c}^\dagger \hat{b},$$

$$(\hat{c}^\dagger \hat{b} + \hat{b}^\dagger \hat{c}) \hat{b} \hat{b}^\dagger \hat{c} = 0.$$

For

$$\hat{F} = \hat{c} \hat{c}^\dagger \hat{b},$$

get

$$[\hat{c} \hat{c}^\dagger \hat{b}, \epsilon_b \hat{b}^\dagger \hat{b} + \epsilon_c \hat{c}^\dagger \hat{c}] = \epsilon_b \hat{c} \hat{c}^\dagger \hat{b},$$

$$\hat{c}\hat{c}^+\hat{b}(\hat{c}^+\hat{b} + \hat{b}^+\hat{c}) = \hat{b}\hat{b}^+\hat{c},$$

$$(\hat{c}^+\hat{b} + \hat{b}^+\hat{c})\hat{c}\hat{c}^+\hat{b} = 0.$$

#### 18.4. Matrix Equation

Using the results obtained so far, it is possible to write the matrix equation

$$\begin{aligned} \hat{L} \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix} &= \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m \\ &= \begin{bmatrix} \epsilon_c \hat{b}\hat{b}^+\hat{c} \\ \epsilon_b \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m \\ &+ \lambda_0 \omega_0 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \\ &\quad \times \sum_{m=0}^{\infty} (m+1) \alpha(n, m+1) |0\rangle\langle 0| \hat{a}^m \\ &+ \lambda_0 \omega_0 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \\ &\quad \times \sum_{m=0}^{\infty} \alpha(n, m-1) |0\rangle\langle 0| \hat{a}^m \\ &+ \omega_0 \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \sum_{m=0}^{\infty} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m. \end{aligned}$$

From the properties of the  $\alpha(n, m)$  get

$$\lambda_0 \omega_0 [(m+1)\alpha(n, m+1) + \alpha(n, m-1)]$$

$$\begin{aligned}
&= \omega_0 [z(m+1)\alpha(n, m+1) + z\alpha(n, m-1)] \\
&= \omega_0 (n - m - z^2)\alpha(n, m).
\end{aligned}$$

Use this to write

$$\begin{aligned}
&\sum_{m=0}^{\infty} \hat{L} \begin{bmatrix} \hat{b}\hat{b}^{\dagger}\hat{c} \\ \hat{c}\hat{c}^{\dagger}\hat{b} \end{bmatrix} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m \\
&= \sum_{m=0}^{\infty} \begin{bmatrix} \epsilon_c + m\omega_0 \\ \epsilon_b + m\omega_0 \end{bmatrix} \begin{bmatrix} \hat{b}\hat{b}^{\dagger}\hat{c} \\ \hat{c}\hat{c}^{\dagger}\hat{b} \end{bmatrix} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m \\
&\quad + \sum_{m=0}^{\infty} \lambda_0 \omega_0 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}\hat{b}^{\dagger}\hat{c} \\ \hat{c}\hat{c}^{\dagger}\hat{b} \end{bmatrix} \\
&\quad \times [(m+1)\alpha(n, m+1) + \alpha(n, m-1)] \\
&\quad \times |0\rangle\langle 0| \hat{a}^m \\
&= \sum_{m=0}^{\infty} \begin{bmatrix} \epsilon_c + m\omega_0 \\ \epsilon_b + m\omega_0 \end{bmatrix} \begin{bmatrix} \hat{b}\hat{b}^{\dagger}\hat{c} \\ \hat{c}\hat{c}^{\dagger}\hat{b} \end{bmatrix} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m \\
&\quad + \sum_{m=0}^{\infty} \lambda_0 \omega_0 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} \hat{b}\hat{b}^{\dagger}\hat{c} \\ \hat{c}\hat{c}^{\dagger}\hat{b} \end{bmatrix} \\
&\quad \times (n - m - z^2)\alpha(n, m) \hat{a}^m.
\end{aligned}$$

For a particular  $m$  get

$$\hat{L} \begin{bmatrix} \hat{b}\hat{b}^{\dagger}\hat{c} \\ \hat{c}\hat{c}^{\dagger}\hat{b} \end{bmatrix} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m$$

$$= \begin{bmatrix} m\omega_0 + \epsilon_c & (n - m - \lambda_0^2)\omega_0 \\ (n - m - \lambda_0^2)\omega_0 & m\omega_0 + \epsilon_b \end{bmatrix} \\ \times \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \alpha(n, m) |0\rangle\langle 0| \hat{a}^m.$$

### 18.5. Matrix Equation for Alternate Basis State

For

$$\hat{\phi} = \hat{F} \sum_{m=0}^{\infty} \alpha(n, m) (a^+)^m |0\rangle\langle 0|,$$

with matrix fermion factor

$$\hat{F} = \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix},$$

similar calculations lead to the matrix equation

$$\hat{L} \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \alpha(n, m) (a^+)^m |0\rangle\langle 0| \\ = \begin{bmatrix} m\omega_0 + \epsilon_c & (n - m - \lambda_0^2)\omega_0 \\ (n - m - \lambda_0^2)\omega_0 & m\omega_0 + \epsilon_b \end{bmatrix} \\ \times \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} \\ \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \alpha(n, m) (a^+)^m |0\rangle\langle 0|.$$

## 18.6. Eigenvalues

The eigenvalues are the roots of the secular equation

$$\begin{vmatrix} m\omega_0 + \epsilon_c & (n - m - \lambda_0^2)\omega_0 \\ (n - m - \lambda_0^2)\omega_0 & m\omega_0 + \epsilon_b \end{vmatrix} = 0; \quad i = 1, 2.$$

They are

$$\lambda_{1,2} = \frac{\epsilon_b + \epsilon_c}{2} + m\omega_0 \pm \sqrt{R},$$

$$\begin{aligned} R &= \left[ \frac{\epsilon_b + \epsilon_c}{2} + m\omega_0 \right]^2 - \epsilon_c \epsilon_b - (\epsilon_b + \epsilon_c)m\omega_0 \\ &\quad - (m\omega_0)^2 + (n - m - \lambda_0^2)^2 \omega_0^2 \\ &= \left[ \frac{\epsilon_b + \epsilon_c}{2} \right]^2 - \epsilon_c \epsilon_b + (n - m - \lambda_0^2)^2 \omega_0^2. \end{aligned}$$

An eigenvector of the secular matrix is found by using an eigenvalue in the matrix equation

$$\begin{bmatrix} \epsilon_c + m\omega_0 - \lambda_i & (n - m - \lambda_0^2)\omega_0 \\ (n - m - \lambda_0^2)\omega_0 & \epsilon_b + m\omega_0 - \lambda_i \end{bmatrix} \begin{bmatrix} X_{1i} \\ X_{2i} \end{bmatrix} = 0.$$

This matrix equation is equivalent to the two simultaneous equations

$$(\epsilon_c + m\omega_0 - \lambda_i)X_{1i}^2 + (n - m - \lambda_0^2)\omega_0 X_{2i}X_{1i} = 0,$$

$$(\epsilon_b + m\omega_0 - \lambda_i)X_{2i}^2 + (n - m - \lambda_0^2)\omega_0 X_{2i}X_{1i} = 0.$$

The nontrivial solution is found from

$$(\epsilon_c + m\omega_0 - \lambda_i)X_{1i}^2 - (\epsilon_b + m\omega_0 - \lambda_i)X_{2i}^2 = 0,$$

which gives the relation of the two components of the eigenvector:

$$X_{2i} = \pm \sqrt{\frac{\epsilon_c + m\omega_0 - \lambda_i}{\epsilon_b + m\omega_0 - \lambda_i}} X_{1i}.$$

Substitution of this relation into the normalization condition

$$X_{1i}^2 + X_{2i}^2 = 1$$

gives the component

$$X_{1i} = \frac{1}{\sqrt{1 + \frac{\epsilon_c + m\omega_0 - \lambda_i}{\epsilon_b + m\omega_0 - \lambda_i}}}.$$

With

$$\begin{bmatrix} \hat{\phi}_b \\ \hat{\phi}_c \end{bmatrix} = \begin{bmatrix} \hat{b}\hat{b}^\dagger\hat{c} \\ \hat{c}\hat{c}^\dagger\hat{b} \end{bmatrix} \alpha(n, m) (a^\dagger)^m |0\rangle\langle 0|,$$

the eigenvectors of the Liouville superoperator are

$$\begin{bmatrix} \hat{\psi}_b \\ \hat{\psi}_c \end{bmatrix} = \begin{bmatrix} X_{11} & X_{21} \\ X_{12} & X_{22} \end{bmatrix} \begin{bmatrix} \hat{\phi}_b \\ \hat{\phi}_c \end{bmatrix}.$$

For a simplified Dirac model with

$$\epsilon_b = \epsilon_c = \epsilon_0,$$

the eigenvalues are

$$\lambda_1 = (n - m + \lambda_0^2)\omega_0,$$

$$\lambda_2 = (n - m - \lambda_0^2)\omega_0.$$

These are the same results obtained in an earlier solution.

The corresponding eigenvectors of the secular matrix are

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix},$$

$$\begin{bmatrix} X_1 \\ X_2 \end{bmatrix}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

The corresponding eigenvectors of the Liouville superoperator are

$$\begin{bmatrix} \hat{\Psi}_1 \\ \hat{\Psi}_2 \end{bmatrix} = \begin{bmatrix} \hat{b}\hat{b}^+\hat{c} + \hat{c}\hat{c}^+\hat{b} \\ \hat{b}\hat{b}^+\hat{c} - \hat{c}\hat{c}^+\hat{b} \end{bmatrix} \alpha(n, m) (\hat{a}^+)^m |0\rangle\langle 0|.$$

## 19. Suggested Topics for Continued Effort

### 19.1. Other Fermion Basis States

Consider some arbitrary imagined system of fermions and bosons. Let  $N$  be the number of fermions in the system at any time, and let  $E$  be the state energy of the Hamiltonian at that time. Assume that transitions of the system between energy levels are possible. Suppose the various  $E$  levels for  $N = 0$  are created by

$$|0, n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle.$$

Suppose various  $E$  levels for  $N = 2$  are created by

$$|\hat{b}\hat{c}, n\rangle = \hat{b}^\dagger \hat{c}^\dagger \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle.$$

Suppose that for  $n = 1$  there are levels for both  $|\hat{b}, n\rangle$  and  $|\hat{c}, n\rangle$ .

Differences in  $E$  levels for the Hamiltonian operator are energy values  $F$  of the Liouville superoperator. These differences can be related to transitions between levels. From a two-fermion  $bc$  level there exist transitions to single-fermion levels for both  $b$  and  $c$ . From a null-fermion level there exist transitions to single-fermion levels for both  $b$  and  $c$ . Thus there should be four different basis eigenvectors for the system.

The Dirac model describes a system resembling the one depicted. The pair of fermion parts of basis states for transitions from a null-fermion level to a single-fermion level have been determined for this model to be

$$\hat{F}_c^{(-)} = \hat{b}\hat{b}^+\hat{c},$$

$$\hat{F}_b^{(-)} = \hat{c}\hat{c}^+\hat{b}.$$

What is the pair

$$\hat{F}_b^{(+)}, \hat{F}_c^{(+)}$$

of fermion parts of basis states for transitions from a single-fermion level to a two-fermion level?

#### 19.2. Green Functions for Summed Basis States

It has been stated that solutions have been obtained for the Einstein, Lee and Dirac models. This claim is something of an overstatement. These exact solutions are eigenvalues of the Liouville superoperators corresponding to simplified Hamiltonian operators containing no summations over states. The remarkable feature of these solutions is that they are exact for all three models.

What would be more useful, however, would be the Green functions for Hamiltonian operators that did contain summations over fermion and boson modes. With such Green functions, it would be possible to determine the thermodynamics of many-particle systems represented by the

more complicated Hamiltonian operators. Obtaining such Green functions would not be a trivial task. One of the necessary steps, for example, would be the calculation of norms from inner products for the summed basis states. Furthermore, the use of summed basis states makes a quadratic solution for exact eigenvalues impossible.

If the Lee model, for example, is generalized to contain summations over boson modes, then the Liouville resolvent method would generate the expanded matrix shown in Table 19.1. In the limit of an infinite number of boson modes, the expanded matrix is infinite. In any case, the expanded matrix contains submatrices of the form shown in Table 19.2. These submatrices resemble the matrix generated for the simplified Lee model with no summation over boson modes. The values of an element in a row  $m$  and column  $n$  of the expanded matrix for the generalized Lee model can be found from Table 19.3.

Table 19.1. Expanded matrix for generalized Lee model.

	$ \hat{c}, 0\rangle$	$ \hat{b}, 0\rangle$	$ \hat{c}, 1\rangle$	$ \hat{b}, 1\rangle$	$ \hat{c}, 2\rangle$	...
$ \hat{c}, 0\rangle$	$\epsilon_c$	0	0	0	0	...
$ \hat{b}, 0\rangle$	0	$\epsilon_b$	$\lambda_0 \omega_0$	0	0	...
$ \hat{c}, 1\rangle$	0	$\lambda_0 \omega_0$	$\epsilon_c + \omega_0$	0	0	...
$ \hat{b}, 1\rangle$	0	0	0	$\epsilon_b + \omega_0$	$\sqrt{2} \lambda_0 \omega_0$	...
$ \hat{c}, 2\rangle$	0	0	0	$\sqrt{2} \lambda_0 \omega_0$	$\epsilon_c + 2\omega_0$	...
...	...	...	...	...	...	...

Table 19.2. Sample submatrix for generalized Lee model.

	$ \hat{b}, n\rangle$	$ \hat{c}, n+1\rangle$
$ \hat{b}, n\rangle$	$\epsilon_b + n\omega_0$	$\sqrt{n+1} \lambda_0 \omega_0$
$ \hat{c}, n+1\rangle$	$\sqrt{n+1} \lambda_0 \omega_0$	$\epsilon_c + (n+1)\omega_0$

Table 19.3. Values of  $a_{mn}$  for generalized Lee model.

	$m = 1, 3, \dots$	$m = 2, 4, \dots$
$n = m + 1$	0	$\sqrt{\frac{n}{2}} \lambda_0 \omega_0$
$n = m$	$\epsilon_c + \frac{(n-1)}{2} \omega_0$	$\epsilon_b + \frac{(n-1)}{2} \omega_0$
$n = m - 1$	$\sqrt{\frac{n}{2}} \lambda_0 \omega_0$	0

Let the expanded matrix for the generalized Lee model be

$$\underline{A} = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1m} & \cdots \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2m} & \cdots \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3m} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ a_{m1} & a_{m2} & a_{m3} & \cdots & a_{mm} & \cdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \end{bmatrix}.$$

The secular matrix is

$$\underline{D} = \underline{A} - \lambda_i \underline{I}, \quad i = 1, 2, \dots$$

The notation used here for an eigenvalue is  $\lambda$  with a subscript that is a nonzero integer, and should not be confused with the notation for a fermion-boson coupling coefficient.

The construction of a Green function, from the eigenvalues associated with a large secular matrix or with a truncated approximation to an infinitely large secular matrix, would require the use of the approximation techniques of the Liouville resolvent method and would be a non-trivial problem. For a specific physical problem, involving actual values of energies and coupling constants, numerical computation would be necessary. An important topic for further investigation is the rate at which a sequence of successively larger truncations converges for particular values of constants in a model.

### 19.3. Differential Operators

The differential representation of boson stepping operators (Saxon 1968:139; Haken 1976:35) permits the eigenvalues of the Hamiltonian operator for a simple harmonic oscillator to be found by easy integration. The questionable use of an "inverse" operator in connection with the so-called "Fock differential representation" leads to a correct result for the eigenvalues of the Hamiltonian operator for a displaced harmonic oscillator. Attempts to use the representation to find eigenvalues of the Liouville superoperator for a displaced harmonic oscillator or for more complicated systems lead to mathematical difficulties that do not so readily succumb to algebraic tricks of dubious validity. Some other way must be used to find such eigenvalues. As it turns out, if suitable basis states are used with the Liouville resolvent method, eigenvalues of the Liouville superoperator can actually be easier to find than eigenvalues of the Hamiltonian operator.

### 19.4. Thermodynamics of Realistic Systems

Simple versions of the Einstein, Lee and Dirac models have been examined. The importance of the eigenvectors and eigenvalues of the  $\hat{L}$  operators for these simple models lies in the connection between the Green functions and the expressions for the energy and thermodynamic functions.

It is well known (Kadanoff and Baym 1962) that the one-

electron Green function will create an expression for the thermal average  $\langle \hat{H} \rangle$  of the Hamiltonian operator, or equivalently of

$$\langle \hat{K} \rangle = \langle \hat{H} \rangle - \mu \langle \hat{N} \rangle,$$

where  $\mu$  is the chemical potential and  $\hat{N}$  is the number operator.

Having an expression for  $\langle \hat{K} \rangle$  and  $\langle \hat{N} \rangle$  for any temperature  $T$  allows an evaluation to be made of the grand canonical potential function  $\Omega(T, V, \mu)$  for a system with a volume  $V$  by using the equation

$$\beta \Omega - (\beta \Omega)_0 = \int_0^\beta \langle \hat{K} \rangle d\beta - \int_0^\beta \beta \frac{\partial \mu}{\partial \beta} \langle \hat{N} \rangle d\beta.$$

The second term on the right-hand side of this equation is present if  $\mu$  is determined as a function of temperature for fixed  $\langle \hat{N} \rangle$ . The familiar symbol

$$\beta \equiv 1/kT$$

is related to the temperature through the Boltzmann constant  $k$ .

The thermal averages that are needed in the expression for  $\langle \hat{K} \rangle$  at each temperature and chemical potential are determined by using the detailed balance condition discussed earlier in this dissertation:

$$\langle A^+ B \rangle = \int \frac{d\omega}{2\pi} f(\omega) A [((\hat{A}, (\omega - \hat{L})^{-1} \hat{B}))].$$

Having a complete set of normalized eigenstates of  $\hat{L}$  from

$$\hat{L}\hat{\Psi}_\alpha = \epsilon_\alpha \hat{\Psi}_\alpha$$

allows the detailed balance equation to be written as

$$\langle \hat{A}^+ \hat{B} \rangle = \sum_\alpha ((\hat{A}, \hat{\Psi}_\alpha)) ((\hat{\Psi}_\alpha, \hat{B})) f(\epsilon_\alpha).$$

Then the determination of the thermal averages of interest requires simply the self-consistent determination of the thermal averages implicitly contained in the inner products  $((\hat{A}, \hat{\Psi}_\alpha))$  and  $((\hat{\Psi}_\alpha, \hat{B}))$ . The complete set of required thermal averages can then be evaluated from the solution of the self-consistent equation of the form just given.

The major contribution of this dissertation has been to study the algebraic foundations for this process as applied to three simple model Hamiltonians. Finding the fermion excitations of the corresponding Liouville superoperator for  $N \rightarrow N + 1$  allows all of the thermal averages that are associated with fermion excitations to be evaluated in the manner described above. The immediate task remaining after this thesis is to study the boson excitations that arise from operating with  $\hat{L}$  on  $\hat{a}$  and  $\hat{a}^+$  in the model Hamiltonians. At that point the thermodynamic self-consistency equations can be solved at various temperatures, and expressions can be determined for an exact self-energy of the systems.

Once the thermodynamics of the simple model Hamiltonians have been determined, it is hoped that the same

algebraic methods can be applied to Hamiltonians that model boson dispersion and many modes.

The application of some of the results of this study should make it feasible to do non-perturbative studies of more realistic model Hamiltonians of the fermion-boson type.

## Literature Cited

- Abraham, D. B.; Robert, M. A. 1980. *J. Phys. A* 13:2229.
- Abrikosov, A. A.; Gorkov, L. P.; Dzyaloshinski, I. E.  
1963. *Methods of quantum field theory in statistical physics*. Silverman, R. A., translator. New York: Dover.
- Adomian, G. 1971. *J. Stat. Phys.* 3:127.
- Anderson, P. W. 1984. *Basic notions of condensed matter physics*. Menlo Park, CA: Benjamin/Cummings.
- Arfken, G. A. 1970. *Mathematical methods for physicists*. 2nd ed. New York: Academic.
- Arons, M. E.; Han, M. Y.; Sudarshan, E. C. G. 1965. *Phys. Rev. B* 137(4):1085.
- Baym, G. [1969] 1974. *Lectures in quantum mechanics*. Corrected 3rd printing. Reading, MA: Benjamin.
- Berger, S. 1983. *Am. J. Phys.* 51(1):10.
- Bjorken, J. D.; Drell, S. D. 1964. *Relativistic quantum mechanics*. New York: McGraw-Hill.
- Bjorken, J. D.; Drell, S. D. 1965. *Relativistic quantum fields*. New York: McGraw-Hill.
- Bleuler, K. 1950. *Helv. Phys. Acta* 23:567.
- Bognar, J. 1974. *Indefinite inner product spaces*.

Berlin: Springer Verlag.

Bowen, S. P. 1975. *J. Math. Phys.* 16(3):620.

Bowen, S. P. 1978. *Phys. Rev. B* 18(7):3400.

Bowen, S. P.; Williams, C. D.; Mancini, J. D. 1984.

*Phys. Rev. A* 30(2):932.

Burington, R. S. 1965. *Handbook of mathematical tables and formulas*. 4th ed. New York: McGraw-Hill.

Byron, F. W.; Fuller, R. W. 1969. *Mathematics of classical and quantum mechanics*. Reading, MA: Addison-Wesley, 2 vols.

Cahill, K. E.; Glauber, R. J. 1969. *Phys. Rev.* 177:1857.

Condon, E. U.; Odabasi, H. 1981. *Atomic structure*. Melbourne, Australia: Cambridge Univ. Press.

Crawford, J. A. 1958. *Nuovo Cimento* 10:6987.

Crowne, F. J. 1983. *J. Phys. C: Solid State Phys.* 16:5563.

Davidson, R.; Kozak, J. J. 1970a. *J. Math. Phys.* 2(1):189.

Davidson, R.; Kozak, J. J. 1970b. *J. Math. Phys.* 2(4):1420.

Dirac, P. A. M. 1942. *Proc. Roy. Soc. (London)* A180:1.

Dirac, P. A. M. 1958. *Quantum mechanics*. Rev. 4th ed. Oxford: Clarendon.

Dirac, P. A. M. 1966. *Lectures on quantum field theory*. New York: Yeshiva Univ. (Belfer Grad. School of Science Monograph Series; No. 3.)

- Dirac, P. A. M. 1978. Directions in physics. New York: Wiley.
- Douglas, D. R. 1982. Lie algebraic methods for particle accelerator theory. Diss. Univ. Maryland. Ann Arbor: UMI. 8308735.
- Dyson, F. 1952. Phys. Rev. 85:631.
- Feenberg, E. 1948. Phys. Rev. 74:206.
- Fetter, A. L.; Walecka, J. D. 1971. Quantum theory of many-particle systems. New York: McGraw-Hill.
- Georgi, H. 1981. Lie algebras in particle physics. Menlo Park, CA: Benjamin/Cummings.
- Gilmore, R. 1974. Lie groups, Lie algebras, and some of their applications. New York: Wiley.
- Goldstein, H. 1980. Classical mechanics. 2nd ed. Reading, MA: Addison-Wiley.
- Green, A. E. S. 1948. Phys. Rev. 73:26.
- Gupta, S. N. 1950. Proc. Phys. Soc. (London) A63:681.
- Gupta, S. N. 1962. Proc. Phys. Soc. (London) A66:129.
- Haken, H. 1973. Quantenfeldtheorie des Festkoerpors. Stuttgart: Teubner.
- Haken, H. 1976. Quantum field theory of solids. Amsterdam: North-Holland.
- Harrison, W. A. 1970. Solid state theory. New York: McGraw-Hill.
- Heisenberg, W. 1957. Nucl. Phys. 4:532.

- Herstein, I. N. 1964. Topics in algebra. Waltham, MA: Blaisdell.
- Hewson, A. C. 1981. J. Phys. C: Solid State Phys. 14:2747.
- Hutson, V.; Pym, J. J. 1980. Applications of analysis. New York: Wiley.
- Inkson, J. C. 1984. Many-body theory of solids: an introduction. New York: Plenum.
- Jackson, J. D. 1975. Classical electrodynamics. 2nd ed. New York: Wiley.
- Jammer, M. 1966. Conceptual development of quantum mechanics. New York: McGraw Hill.
- Jordan, T. F. 1969. Linear operators for quantum mechanics. New York: Wiley.
- Judd, B. R. 1962. Operator techniques in atomic spectroscopy. New York: McGraw-Hill.
- Judd, B. R.; Elliot, J. P. 1970. Topics in atomic and nuclear theory. Univ. of Canterbury, N. Z.
- Kadanoff, L. P.; Baym, G. 1962. Quantum statistical mechanics. New York: Benjamin.
- Kadanoff, L. P.; Martin, P. L. 1961. Phys. Rev. 124:670.
- Kaempffer, F. 1965. Concepts in quantum mechanics. New York: Academic.
- Killingbeck, J.; Cole, G. H. A. 1971. Mathematical techniques and physical applications. New York: Academic.

- Kirzhnits, D. A. 1967. Field theoretical methods in many-body systems. Brink, D. M., ed. Meadows, A. J., translator. Oxford: Pergamon.
- Krein, M. G.; Langer, G. R. 1964. Soviet Math Dokl. 4:1236. From: 1963. Dokl. Akad. Nauk. 4(5):39.
- Liboff, R. L. 1980. Introductory quantum mechanics. Oakland, CA: Holden-Day.
- Lee, T. D.; Wick, G. C. 1969. Nucl. Phys. B9:209.
- Lonke, A. 1971. J. Math. Phys. 12:2422.
- Mahan, G. D. 1981. Many-particle physics. New York: Plenum.
- Mandl, F. 1959. Introduction to quantum field theory. New York: Wiley-Interscience.
- Mandl, F.; Shaw, G. 1985. Quantum field theory. New York: Wiley.
- March, N. H.; Young, W. H.; Sampanthar, S. 1967. The many-body problem in quantum mechanics. Cambridge: Univ. Press.
- Masson, P. 1970. In: Baker, G. A., Jr.; Gammel, J. L.; eds. Pade approximant in theoretical physics. New York: Academic.
- Mathews, J.; Walker, R. L. 1970. Mathematical methods of physics. 2nd ed. Menlo Park, CA: Benjamin/Cummings.
- Merzbacher, E. 1970. Quantum mechanics. 2nd. ed. New York: Wiley.

- Messiah, A. 1968. Quantum mechanics. 2nd ed. Temmer, G. M., translator. New York: Wiley, 2 vols.
- Miller, W., Jr. 1968. Lie theory and special functions. New York: Academic. (Mathematics in science and engineering; vol. 43.)
- Mohling, F. 1982. Statistical mechanics. New York: Wiley.
- Nagy, K. L. 1960. Nuovo Cimento Suppl. 17:921.
- Nagy, K. L. 1966. State vector spaces with indefinite metric in quantum field theory. Groningen: Noordhoff.
- Nagy, K. L. 1970. Acta Phys. Acad. Sci. Hungar. 29:251.
- Pais, A.; Uhlenbeck, G. E. 1950. Phys. Rev. 79:145.
- Pathria, R. K. 1972. Statistical mechanics. New York: Pergamon.
- Pauli, W. 1943. Rev. Mod. Phys. 15:175.
- Pauli, W.; Villars, F. 1949. Rev. Mod. Phys. 21:434.
- Powell, J. L.; Crasemann, B. 1961. Quantum mechanics. Reading, MA: Addison-Wesley.
- Rickayzen, G. 1980. Green's functions and condensed matter. London: Academic.
- Riesz, F.; Nagy, B. Sz. 1955. Functional analysis. New York: Unger.
- Rivier, N.; Coe, R. J. 1977. J. Phys. C: Solid State Phys. 10:4471.
- Roman, P. 1965. Advanced quantum theory. Reading, MA: Addison-Wesley.

- Sakurai, J. J. 1967. Advanced quantum mechanics. Reading, MA: Addison-Wesley.
- Saxon, D. S. 1968. Elementary quantum mechanics. San Francisco: Holden-Day.
- Schwarzschild, B. M. 1985. Phys. Today, Aug.:17.
- Schweber, S. S. 1961. An introduction to relativistic quantum field theory. Evanston, IL: Row, Peterson.
- Simmons, G. F. 1963. Introduction to topology and modern analysis. New York: McGraw-Hill.
- Snygg, J. 1981. Am. J. Phys. 50(10):906.
- Stolze, J.; Brandt, U. 1983. J. Phys. C: Solid State Phys. 16:5617.
- Symon, K. 1971. Mechanics. 3rd ed. Reading, MA: Addison-Wesley.
- Talman, J. D. 1968. Special functions. Reading, MA: Benjamin.
- ter Haar, D. 1985. Rev. of Inkson, J. C., Many-body theory of solids. Phys. Today, May:85.
- Wan, Z. X. 1975. Lie algebras. New York: Pergamon.
- Watson, G. N. 1952. A treatise on the theory of Bessel functions. 2nd ed. Cambridge: Cambridge Univ. Press.
- Whittaker, E. T.; Watson, G. N. 1962. A course of modern analysis. 4th ed. New York: Cambridge Univ. Press.
- Ziman, J. M. 1960. Theory of transport phenomena in solids. Oxford: Oxford Univ. Press.

Ziman, J. M. 1969. Elements of advanced quantum theory.

Cambridge: Cambridge Univ. Press.

Zubarev, D. 1960. Usp. Fiz. Nauk. 71:71. [1960. Sov.

Phys. Usp. 3:320.]

**The vita has been removed from  
the scanned document**

Bressler, B. L. 1986. An Application of the Liouville  
 Resolvent Method to the Study of Fermion-Boson  
 Couplings. Physics dept., Va. Tech.

Corrigenda as of 23 November 1986 are as follows: (Of  
 these errors, only the ones on pages x and 6 appear in  
 publication 8620592 of University Microfilms International.)

Page	Line	Erratum	Correction
ii	12	. Implementation	. Implementation
ii	16	states. These	states. These
x	12	Weh-Ming	Wei-Ming
6	9	1976; Haken 1976;	1976;
59	6	$\langle [\hat{A}(t), \hat{B}(t')] ]_{\eta} \rangle$	$\langle [\hat{A}(t), \hat{B}(t')] \rangle$
60	3	$\langle [\hat{A}(t), \hat{B}(t')] ]_{\eta} \rangle$	$\langle [\hat{A}(t), \hat{B}(t')] \rangle$
60	4	$\langle [\hat{A}(t), \hat{B}(0)] ]_{\eta} \rangle$	$\langle [\hat{A}(t), \hat{B}(0)] \rangle$
60	16	-1	+1
60	17	+1	-1
61	6	G(t,0)	G(t, 0)
61	10	- $\eta$	$[(\eta - 1) - (\eta + 1)i]/2$
61	10	$\langle [\hat{A}(t), \hat{B}^+(0)] \rangle_{\eta}$	$\langle [\hat{A}(t), \hat{B}^+(0)]_{\eta} \rangle$ .
61	11	minus	plus
61	19	one	minus one
61	22	one	minus one
62	14	one	minus one
65	13	$e^{i\hat{H}t/\hbar}$	$e^{i\hat{H}t/\hbar}$
135	14	$[\hat{a}^a, (\hat{a}^+)^s \hat{a}^s]$	$[\hat{a}^q, (\hat{a}^+)^s \hat{a}^s]$