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A SYSTEMATIC STUDY AND APPLICATIONS OF THE EIGENVALUE PROBLEM FOR QUADRATIC HAMILTONIANS

A Dissertation

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of Doctor of Philosophy

in

The Department of Physics and Astronomy

by James Lannis Roberts B.S., Louisiana State University, 1963 January, 1968

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ABSTRACT

A systematic procedure is developed for solving the eigenvalue problem for a broad class of Hamiltonian operators containing no terms higher than quadratic in generalized coordinates and their conjugate momenta. The development is oriented toward practical applications in the area of the many-body problem. The procedure accomplishes a canonical reduction of such a Hamiltonian to the form of the Hamiltonian for a collection of noninteracting bosons, with the eigenvalues of the Hamiltonian expressed in terms of the solutions to a single secular equation.

Application of the results to systems of interacting identical bosons is discussed, including a presentation of a useful calculational technique. The procedures developed are illustrated by detailed treatments of two specific problems of interest in physics.

The first problem considered is an exactly solvable separable potential model of particle field theory. This problem consists of the description of a collection of light bosons interacting with an infinitely heavy boson via a simple separable potential. Interest in this problem centers on its use as a test case for approximation techniques to be used on more complicated systems.

The second and more realistic problem investigated is the polaron problem of solid state physics. This problem involves the

iv

description of the motion of a single conduction electron within an ionic solid. The polaron consists of the conduction electron together with its self-induced polarization field. The polaron problem is of interest not only because of its value in solid state physics, but also because it, too, is useful as a testing ground for approximation techniques.

Finally, broad applicational aspects of the procedures developed are discussed.

CHAPTER 1

INTRODUCTION

(1,1) Objectives

The behavior of many physical systems may be described or approximated by a (Hermitian) Hamiltonian operator which contains no terms of order higher than quadratic in generalized coordinates and their canonically conjugate momenta. The general form of such a Hamiltonian is:

$$H = H_0 + H_1 + H_2$$

(1,1;1)

with

$$H_{i} = \sum_{j} \left[c_{j} p_{j} + d_{j} q_{j} \right]$$

(1,1;2)

and

$$H_{2} = \frac{1}{2} \sum_{jj'} \left[u_{jj'} P_{j} P_{j}, + w_{jj'} q_{j} q_{j'} + Z_{jj'} (P_{j} q_{j'} + q_{j} P_{j'}) \right],$$
(1,1;3)

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where j and j' are indices running 1,2,3,...,N (In some applications the limit $N \rightarrow \infty$ is taken.); q_j is a generalized coordinate and p_j is its conjugate momentum; u_{jj'}, w_{jj'}, and z_{jj'} are real, symmetric functions of j and j'; c_j and d_j are real functions of j; and H_o is a real constant. Consideration will be restricted to treatment of the broad class of physical systems which possess a ground state and whose Hamiltonian may be cast into the preceding form with $\sum_{ij'} u_{jj'} p_j p_{j'} > 0$.

A trivial example of (1,1;1) is a Hamiltonian of the form

$$= \sum_{j} \left[\frac{1}{2m_{j}} P_{j}^{2} + \frac{1}{2} m_{j} \omega_{j}^{2} q_{j}^{2} \right] + H_{o},$$
(1,1;4)

where m_j and w_j are real positive functions of j. If $H_0 = 0$, then H is of the form of the Hamiltonian for a set of N noninteracting simple harmonic oscillators for which the jth one has mass m_j and an angular frequency w_i . If

$$H_{o} = -\frac{\pi}{2} \sum_{j} \omega_{j},$$

then $\not\models$ has the form of the Hamiltonian of a collection of bosons of N types for which the jth type has an energy of hw_j. There are other interesting physical systems whose Hamiltonians may be approximated by (1,1;1). Notable examples, such as liquid helium,¹ the phonon field of a polaron,² and the π -meson field of a nucleon,³ may be selected from various fields of physics.

(1,1)

A central part of a quantum mechanical description of a system is finding the eigenvalues and eigenfunctions of its Hamiltonian. The primary objective of the present research is to prescribe a systematic and practical procedure for finding the eigenvalues of the Hamiltonian (1,1;1). The secondary objective is to illustrate the procedure with physically interesting examples. The final objective is to indicate a powerful method of employing the procedure to systems whose Hamiltonian may be approximated by one of the form of (1,1;1).

(1,2) Method

It turns out, as will be demonstrated, that it is possible to define "new" generalized coordinates, Q_j (j = 1,2,...,n), and corresponding conjugate momenta, P_j , as linear combinations of the "old" ones (the q_j's and the p_j's) occurring in (1,1;1) through (1,1;3) in such a way that when H is expressed in terms of them, the result is in the so called "completely reduced" form

$$H = \frac{1}{2} \sum_{j} \left[P_{j}^{2} + \Omega_{j}^{2} Q_{j}^{2} \right] + E_{o}, \qquad (1.2:1)$$

where E_0 and Ω_1^2 , Ω_2^2 ,..., Ω_N^2 are real constants to be determined. In view of this result, the eigenvalues of H are well known. Unless all of the Ω_j^2 's are positive, H will not possess a ground state, contrary to the previously stated restriction. Hence $\Omega_j \equiv + \int_{\Omega_j^2}^{\Omega_j^2}$ (j = 1, 2, ..., N) is positive; and the eigenvalues of H are given by

3 (1,1) ∝ 0

(1,2)

$$= \sum_{n_{1}, n_{2}, \dots, n_{N}} = \sum_{j} \left[\hbar \Omega_{j} (n_{j} + \frac{1}{2}) \right] + E_{o,j}$$
(1,2;2)

where $n_j = 0, 1, 2, ...$ The eigenfunctions of H are similarly well known functions of $Q_1, Q_2, ..., Q_N$, depending parametrically upon $\Omega_1, \Omega_2, ..., \Omega_N$. Accordingly, the primary objective may be reduced to finding a practical procedure for determining the Ω_j 's and E_0 .

The reduction of the Hamiltonian H to the completely reduced form (1,2;1) will be handled in two stages. In the first stage, new coordinates, q_i 's, and conjugate momenta, p_i 's, will be defined, in terms of which H will have the form

$$H = \frac{1}{2} \sum_{jj'} \left[u_{jj'} P_{j}' P_{j}' + V_{jj'} q_{j}' q_{j}' \right] + E_{o,j}$$
(1,2;3)

where v_{jj} , and E_0 are to be specified. The first stage will involve two steps. The first one will eliminate from the Hamiltonian terms involving products of a coordinate and a momentum, called "mixed products." The second step will eliminate terms linear in coordinates and momenta. In the second stage, the "final" coordinates, Q_j 's, and conjugate momenta, P_j 's, will be defined in terms of the q_j ''s and the p_j ''s, occurring in (1,2;3), so that when H is written in terms of them, the result is (1,2;1), with $\Omega_1, \Omega_2, \dots, \Omega_N$ determined. The second stage will involve three steps. First, terms involving products of different momenta ("p-p cross terms") will be eliminated.

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Next, the coefficients of terms proportional to the square of a momentum will be rendered all equal to unity by a simple, so called "scaling transformation." Finally, terms containing products of different coordinates ("q-q cross terms") will be eliminated. From the considerations involved in stage two, a single secular equation will be derived to determine $\Omega_1, \Omega_2, \dots, \Omega_N$.

(1,3) Notation

The symbols j and j' are reserved to denote indices running 1,2,3,...,N.

The following convention will be used. If v_j is a singly subscripted symbol, then, the symbol, v, obtained by dropping the subscript is reserved to denote the matrix

$$V \equiv \begin{pmatrix} V_1 \\ V_2 \\ \vdots \\ V_N \end{pmatrix}.$$
(1,3;1)

Similarly, if t_{ii} is a doubly subscripted symbol, then

$$t = \begin{pmatrix} t_{11} & t_{12} & \cdots & t_{1N} \\ t_{21} & t_{22} & \cdots & t_{2N} \\ \vdots & \vdots & \ddots & \vdots \\ t_{N1} & t_{N2} & \cdots & t_{NN} \end{pmatrix}$$
(1,3;2)

The transpose of a matrix t will be denoted by \tilde{t} . The unit NxN matrix will be denoted by e.

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(1, 2)

Square brackets with exterior subscripts are used to denote the set of all quantities obtained by substituting all possible values of the exterior subscript into the enclosed function of the exterior subscript. (Example: If i has possible values 1 and 2, then $[f_{ii}]_i = f_{1i}, f_{2i}$.)

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(1,3)

CHAPTER 2

REDUCTION

(2,1) Elimination of Mixed Products and Linear Terms

Recall equations (1,1;1) through (1,1;3):

$$H = H_{0} + H_{1} + H_{2}$$
(2,1;1)

$$H_{1} = \sum_{j} \left[C_{j} P_{j} + d_{j} q_{j} \right]$$
(2,1;2)

$$H_{2} = \frac{1}{2} \sum_{j,j'} \left[U_{jj'} P_{j} P_{j}, + W_{jj'} q_{j} q_{j'} + Z_{jj'} (P_{j} q_{j}, + q_{j} P_{j}) \right] .$$
(2,1;3)

To eliminate mixed products, define canonically conjugate coordinates q^{μ} and momenta p^{μ} by the equations

$$P = P'' + g q''$$

$$q = q'',$$
(2,1;4)

where

$$g = -u^{-1}Z$$

(2,1;5)

Substitution of (2,1;4) into (2,1;1) through (2,1;3) and use of (2,1;5) yield

$$H = H_0 + H_1' + H_2',$$
 (2,1;6)

with

$$H'_{i} = \sum_{j} \left[c_{j} P_{j}'' + f_{j} q_{j}'' \right]$$
(2,1;7)

and

$$H_{2} = \frac{1}{2} \sum_{j,j'} \left[u_{jj'} P_{j'}'' P_{j'}'' + V_{jj'} q_{j}'' q_{j'}'' \right],$$

(2,1;8)

where

$$f = d + \tilde{g}c$$

(2,1;9)

and \boldsymbol{v} is the symmetric matrix

$$V = W + Zg$$
.

(2,1;10)

To eliminate linear terms, define canonically conjugate coordinates q' and momenta p' by

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$$p'' = p' + l$$

$$q'' = q' + m,$$

where

$$L = -2 UC$$

m = -2 Vf.

(2,1;12)

(2,1;11)

Substitution of (2,1;11) into (2,1;6) through (2,1;8) and use of (2,1;12) yield

$$H = \frac{1}{2} \sum_{jj'} \left[u_{jj}, P'_{j}P'_{j} + V_{jj}, q'_{j}q'_{j} \right] + E_{o}$$
(2,1;13)

with

$$E_{o}=H_{o}+\tilde{c}\ell+\tilde{f}m+\frac{1}{2}[\tilde{\ell}u\ell+\tilde{m}vm],$$
(2,1;14)

where equations (2,1;5), (2,1;9), (2,1;10), and (2,1,12) express v, &, m, and f in terms of quantities occurring in the original expression for H, given by (2,1;1) through (2,1;3). (2,2) Completion of the Reduction

Since the matrix u is real and symmetric, there exists⁴ an orthogonal matrix, t, such that the matrix

u'= tut

is diagonal; i.e.,

$$\mathcal{U}' = \begin{pmatrix} S_{11}^{2} & S_{22}^{2} \\ S_{22}^{2} & S_{NN} \end{pmatrix},$$

(2, 2; 2)

(2, 2; 1)

where, since u is positive definite, $s_{jj} \equiv + \left(s_{jj}^2\right)^2$ must be real and positive. Define conjugate coordinates Q' and corresponding momenta P' by

$$p' = t P''$$

 $q' = t Q''.$
(2,2;3)

Substitution of (2,2;3) into (2,1;13) and use of (2,2;1) and (2,2;2) give

$$= \frac{1}{2} \sum_{jj'} \left[s_{jj}^{2} P_{j}^{"2} \delta_{jj'} + V_{jj'} Q_{j}^{"} Q_{j'}^{"} \right] + E_{o},$$

$$(2,2;4)$$

*For proof that P'' and Q'' are conjugate, see Appendix (Al,l).

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(2,2)

(2,2)

11

where

$$v' = \tilde{t}vt.$$

(2,2;5)

Notice that p-p cross terms have been eliminated from (2,2;4).

Next, define canonically conjugate coordinates, Q', and momenta P' by

 $P_{j}^{\prime\prime} = \frac{1}{S_{jj}} P_{j}^{\prime}$ $Q_{j}^{\prime\prime} = S_{jj} Q_{j}^{\prime}.$ (2,2;6)

For reference, let

$$S = + [U'] = \begin{pmatrix} S_{11} & O \\ S_{22} & O \\ O & S_{NN} \end{pmatrix};$$
 (2,2;7)

and note that the unit NxN matrix, e, may be written as

e = S' u S' (2,2;8)

Substitution of (2,2;6) into (2,2;4) gives

$$H = \frac{1}{2} \sum_{j,j'} \left[P_{j'}^{2} \delta_{jj'} + V_{jj'}^{"} Q_{j}' Q_{j'}' \right] + E_{o}, \qquad (2,2;9)$$

where

Notice that the coefficient of P_j ² in (2,2;9) is unity for all j.

Finally, since v'' is real and symmetric, there exists⁴ an orthogonal matrix, r, such that the matrix $\tilde{r}v''r$ is diagonal. Thus

$$\nabla''' \equiv \widetilde{\Gamma} \nabla'' \Gamma \equiv \begin{pmatrix} \Omega_1^2 & 0 \\ \Omega_2^2 & \Omega_3^2 \\ 0 & \Omega_3^2 \\ 0 & \Omega_N^2 \end{pmatrix}.$$
 (2,2;11)

Define final coordinates Q and corresponding momenta P by \star

$$P'=rP$$

 $Q'=rQ$ (2,2;12)

Substitution of (2,2;12) into (2,2;9) and use of (2,2;11) yield the desired completely reduced form.

$$H = \frac{1}{2} \sum_{j} \left[P_{j}^{2} + \Omega_{j}^{2} Q_{j}^{2} \right] + E_{o}.$$
(2,1;13)

Notice that the deriviation of this result requires the restriction that u be positive definite. The further restriction that H possess a ground state will be met if and only if all of the Ω_j^2 's are positive which in turn is equivalent to the requirement that v be positive definite.

*For proof that P and Q are conjugate, see Appendix (A1,1).

A useful and convenient single secular equation for the determination of $\Omega_1^2, \Omega_2^2, \ldots, \Omega_N^2$ may now be derived from the preceeding results. Let

$$y = t s r.$$
 (2,2;14)

The equation

$$\prod_{j} \left[\Omega^2 - \Omega_j^2 \right] = O \tag{2,2;15}$$

clearly yields exactly the solutions $\Omega^2 = \Omega_1^2, \Omega_2^2, \dots, \Omega_N^2$. This equation may be reexpressed as follows by employing equations (2,2;11), (2,2;8) (2,2;10), (2,2;5), (2,2;1), and (2,2;14) and by recalling that s is diagonal and that r and t are othogonal:

$$O = \prod_{j} \left[\Omega^{2} - \Omega_{j}^{2} \right]$$

= $\| \Omega^{2} e^{-ev'''} \|$
= $\| \Omega^{2} e^{-(r'er)(r'v''r)} \|$
= $\| \Omega^{2} e^{-(r's''v's''r')(rsv'sr)} \|$
= $\| \Omega^{2} e^{-(r's''t''uts''r)(r'st''vtsr)} \|$
= $\| \gamma^{-i} [\Omega^{2} e^{-uv}] y \|$
= $\| \Omega^{2} e^{-uv} \|$

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(2,2)

Thus, the solutions of the secular equation

$$\|\Omega^2 e - uv\| = 0$$
(2,2;16)

are exactly $\Omega^2 = \Omega_1^2, \Omega_2^2, \dots, \Omega_N^2$.

(2,3) Resume of Results

A canonical linear transformation has been found which reduces a Hamiltonian of the form

$$H = H_{o} + \sum_{j} \left[c_{j} P_{j} + d_{j} q_{j} \right]$$

+ $\frac{1}{2} \sum_{jj'} \left[u_{jj'} P_{j} P_{j}, + W_{jj'} q_{j} q_{j'}, + Z_{jj'} (P_{j} q_{j'}, + q_{j} P_{j'}) \right]$
(2,3;1)

to the form

$$H = \frac{1}{2} \sum_{j} \left[P_{j}^{2} + \Omega_{j}^{2} Q_{j}^{2} \right] + E_{o}.$$
(2,3;2)

In this result, the set $\{\Omega_1^2, \Omega_2^2, \dots, \Omega_N^2\}$ is the set of solutions of the secular equation,

$$\|\Omega^2 e - uv\| = 0, \qquad (2,3;3)$$

where v is given by

(2,3)

(2,3;4)

(2,3;7)

$$V = W + Z g$$

and

$$g = -U^{-1}Z$$
. (2,3;5)

Moreover, E_{o} is given by

$$E_{\circ} = H_{\circ} + \tilde{c}l + \tilde{f}m + \frac{1}{2} [\tilde{l}ul + \tilde{m}vm], \qquad (2,3;6)$$

where

$$\begin{cases} l = -2uc \\ m = -2vf \\ f = d + \tilde{g}c. \end{cases}$$

The results summarized in (2,3;1) through (2,3;3) are valid if and only if either u or v is positive definite. However, according to the original statement of the problem, both u and v are positive definite.

(2,4) Translation to Second Quantization Language

It is desirable for applicational purposes to express the preceding results for obtaining the eigenvalues of H in the language of second quantization. Such a reexpression of results will be accomplished

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in a rather direct manner in the present section.

The Hamiltonian, H, given in terms of p and q by (2,3;1) may be rewritten as

$$H = h_{o} + h_{i} + h_{2}$$
, (2,4;1)

with

.

$$h_{j} = \sqrt{\frac{\pi}{2}} \sum_{j} \left[\eta_{j} a_{j} + \eta_{j}^{*} a_{j}^{\dagger} \right]$$
(2,4;2)

and

$$h_{2} = \frac{\pi}{4} \sum_{jj'} \left\{ (\alpha_{jj'} - i\beta_{jj'}) a_{j} a_{j}, + (\alpha_{jj'} + i\beta_{jj'}) a_{j}^{\dagger} a_{j}^{\dagger}, + 2\delta_{jj'} a_{j}^{\dagger} a_{j}, \right\}, \qquad (2,4;3)$$

wherein

$$\begin{array}{l} \eta = c - id \\ \alpha = w - u \\ \vartheta = w + u \\ \beta = 2 z \\ h_o = H_o + \sum_{j} \vartheta_{jj} \end{array}$$

and

$$a = f_{2\pi}^{+} (q + ip)$$

$$a^{+} = f_{2\pi}^{+} (q - ip).$$

(2,4;4)

(2,4;5)

(2,4)

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In view of (2,4;5), a_j^{\dagger} and a_j satisfy the commutation rules,

$$\begin{bmatrix} a_{j}, a_{j'}^{\dagger} \end{bmatrix} = \delta_{jj},$$

$$\begin{bmatrix} a_{j}, a_{j'} \end{bmatrix} = \begin{bmatrix} a_{j}^{\dagger}, a_{j'}^{\dagger} \end{bmatrix} = 0,$$

$$(2,4;6)$$

appropriate for creation and distruction operators respectively.

Similarly, H, given in terms of P and Q by (2,3;2), may be rewritten as

$$H = \sum_{j} \left[\hbar \Omega_{j} A_{j}^{\dagger} A_{j} \right] + E_{a}^{\prime}, \qquad (2,4;7)$$

where

$$A_{j} = \frac{1}{12\pi\Omega_{j}} \left(\Omega_{j}Q_{j} + iP_{j} \right)$$

$$A_{j}^{\dagger} = \frac{1}{12\pi\Omega_{j}} \left(\Omega_{j}Q_{j} - iP_{j} \right)$$

$$(2,4;8)$$

and where, in view of (2,3;3) through (2,3;7) and (2,4;4), $\Omega^2 = \Omega_1^2, \Omega_2^2, \dots, \Omega_N^2 \text{ are the roots of the secular equation}$

$$\|\Omega^2 e - uv\| = 0 \tag{2.4.9}$$

and

$$\begin{split} \Xi_{o}^{\prime} &= h_{o} - \left[\frac{\hbar}{4} \sum_{j} \delta_{jj}\right] + \left[\frac{\hbar}{2} \sum_{j} \Omega_{j}\right] \\ &+ \widetilde{c} \mathcal{L} + \widetilde{f} m + \frac{1}{2} \left[\widetilde{\mathcal{L}} u \mathcal{L} + \widetilde{m} v m\right], \end{split}$$

$$(2,4;10)$$

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(2,4)

wherein

$$C = \frac{1}{2} (\eta + \eta^{*})$$

$$f = \frac{1}{2} \widetilde{m} (\eta + \eta^{*}) + \frac{1}{2} (\eta - \eta^{*})$$

$$u = \frac{1}{2} (\vartheta - \alpha)$$

$$v = \frac{1}{2} [(\vartheta + \alpha) - \wp (\vartheta - \alpha)^{-1} \wp]$$

$$l = -2 v f$$

$$m = -2 u C.$$

(2,4;11)

Since, according to (2,4;8), the A_j^{\dagger} 's and the A_j 's satisfy the creation and distruction operator commutation rules,

$$\begin{bmatrix} A_{j}, A_{j}^{\dagger} \end{bmatrix} = \delta_{jj},$$

$$\begin{bmatrix} A_{j}, A_{j'} \end{bmatrix} = \begin{bmatrix} A_{j}^{\dagger}, A_{j'}^{\dagger} \end{bmatrix} = 0; \qquad (2,4;12)$$

then, the eigenvalues of a Hamiltonian of the form of (2,4;1) with (2,4;2) and (2,4,3) are given directly in terms of the coefficients occurring in it by

$$E_{n_{i},n_{2},...,n_{N}} = \sum_{j} \hbar \Omega_{j} n_{j} + E_{o}, \qquad (2,4;13)$$

where $n_j = 0, 1, 2, 3, \dots, \Omega_j = + \sqrt{\Omega_j^2}$, and where E_0' and $\Omega_1^2, \Omega_2^2, \dots, \Omega_N^2$ are determined by (2,4;9) through (2,4;11).

These results hold if and only if both u and v are positive definite.

CHAPTER 3

APPLICATIONS

(3,1) Introduction and Orientation

Hitherto the discussion has centered about a systemization of procedures for canonically reducing a quadratic Hamiltonian. It is the purpose of this chapter to illustrate the application of these systematic procedures to specific physically interesting problems.

The physical systems which will be used for illustration are systems of identical, interacting bosons. The discussion of these systems will be cast in the language of second quantization. The quantum mechanical states of such a system are to be described in terms of the single particle states given by

$$\Psi_{\vec{k}}(\vec{r}) = \frac{1}{1V} e^{i\vec{k}\cdot\vec{r}},$$

where \vec{r} is the coordinate vector, $V = L^3$ is a cubic normalization volume, and \vec{k} is the wavevector of a particle in the state $\psi_{\vec{k}}(\vec{r})$. The imposition of periodic boundary conditions on the surface of the normalization volume requires that the ith rectangular component of \vec{k} satisfy

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(3,1)

(3, 1; 1)

$$k_i = \frac{2\pi}{L} n_i,$$

where

$$n_i = 0, \pm 1, \pm 2, \cdots$$

and

In the final analysis, the limit $L \rightarrow \infty$ is taken so that \vec{k} becomes a continuous variable and

$$\sum_{\vec{k}} \longrightarrow \frac{\vec{V}}{8\pi^3} \int d^3\vec{k}$$

all \vec{k} -space (3,1;2)

In Chapters 1 and 2, the indices employed have a finite domain of N elements. For the applications which follow, it will be assumed tacitly that the results are valid in the limit $N \rightarrow \infty$. This point will not be belabored here.

(3,2) A Calculational Technique

Prior to focusing attention on specific physical systems, it will be advantageous to investigate a calculational method.⁵ Suppose it is desired to evaluate 20

(3,2;1)

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$$\mathfrak{F} = \sum_{\Omega} G(\Omega) - \sum_{\overline{k}} G(\omega(k)),$$

where G is some function of a single complex variable and where the first summation is over the set of all solutions for Ω of the secular equation

$$\left\| \left[\Omega - \omega(\vec{k}) \right] \delta_{\vec{k}\vec{k}'} - \frac{1}{\nabla} F(\vec{k}) * F(\vec{k}') \right\| = 0.$$

$$(3.2:2)$$

In equations (3,2;1) and (3,2;2), \vec{k} and \vec{k}' are indices whose domain is given by (3,1;1); $\omega(\vec{k})$ is a real function of \vec{k} ; and

$$F(\vec{k}) * F(\vec{k}) = \sum_{i=1}^{n} F_i(\vec{k}) F_i(\vec{k}),$$
 (3.213)

wherein n is a finite (preferably small) positive integer and $F_i(\vec{k})$ is a real function of \vec{k} and i. Since $\omega(\vec{k}) \delta_{\vec{k}\vec{k}'} + F(\vec{k}) * F(\vec{k}')$ is real and symmetric, the solutions for Ω of equation (3,2;2) are real. It will be assumed, moreover, that the greatest lower bound, ω_o , of the union of $[\Omega]_{\Omega}$ with $[\omega(\vec{k})]_{\vec{k}}$ is a positive number.

In a complex plane, z, consider a path, P, which encloses the locus, L, of all points, z, on the real axis such that $z \ge w_0$.

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If G(z) is analytic everywhere within and on the closed contour P, then

$$g = \sum_{n} \frac{1}{2\pi i} \oint_{p} \frac{G(z)}{z - n} dz - \sum_{\vec{k}} \frac{1}{2\pi i} \oint_{p} \frac{G(z)}{z - \omega(\vec{k})} dz$$
(3,2;4)

$$= \frac{1}{2\pi i} \oint_{P} dz G(\overline{z}) \left[\sum_{\Omega} \frac{1}{\overline{z} - \Omega} - \sum_{\overline{k}} \frac{1}{\overline{z} - \omega(\overline{k})} \right].$$
(3,2;5)

For all z not on the locus L indicated in the accompanying diagram, define

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(3,2)

$$J(z) \equiv \prod_{k} (z - \Omega)$$

$$= \left\| \left[z - \omega(\vec{k}) \right] \delta_{\vec{k} \cdot \vec{k}'} - \frac{1}{\nabla} F(\vec{k}) * F(\vec{k}) \right\|,$$

$$(3,2;6)$$

$$J_{o}(z) \equiv \prod_{k} \left[z - \omega(\vec{k}) \right]$$

$$= \left\| \left[z - \omega(\vec{k}) \right] \delta_{\vec{k} \cdot \vec{k}'} \right\|,$$

(3,2;7)

• .

and

$$\Gamma(z) \equiv \frac{J(z)}{J_{o}(z)} = \frac{\prod_{k} (z - \Omega)}{\prod_{k} [z - \omega(\overline{k})]}$$
(3,2;8)

Thus from (3,2;5) and (3,2;8), it follows that

$$g = \frac{1}{2\pi i} \oint_{P} d \Xi G(\Xi) \frac{d}{d\Xi} \mathcal{L}_{og} \Gamma(\Xi), \qquad (3,2;9)$$

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(3,2)

.

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where

$$\log Z = \log |Z| + i \log Z$$
 (3,2;10)

$$-\pi < \operatorname{arg} Z \leq +\pi.$$
(3,2;11)

Integration by parts once yields

$$g = -\frac{1}{2\pi i} \oint_{P} dz G'(z) \partial_{og} \Gamma(z).$$
(3,2;12)

By definition of $\Gamma(z)$ in (3,2;8), (3,2;7), and (3,2;6), one may write

$$\begin{split} \Gamma(z) &= \frac{1}{\prod_{k} \left[z - \omega(\vec{k}) \right]} \left\| \left[z - \omega(\vec{k}) \right] \delta_{\vec{k} \cdot \vec{k}} - \frac{1}{\nabla} F(\vec{k}) * F(\vec{k}) \right\| \\ &= \left\| \delta_{\vec{k} \cdot \vec{k}} - \frac{1}{\nabla} \frac{F(\vec{k}) * F(\vec{k})}{\left[z - \omega(\vec{k}) \right] \left[z - \omega(\vec{k}) \right]} \right\|. \end{split}$$

Let

•

$$Q_{i}(\vec{k}) = \frac{1}{1\sqrt{1}} \frac{F_{i}(\vec{k})}{1/2}$$

Then, use of (3,2;3) yields

$$\Gamma(z) = \left\| \delta_{\vec{k}\vec{k}'} - \sum_{i} Q_{i}(\vec{k}) Q_{i}(\vec{k}') \right\|$$

(3,2)

or

$$T_{(Z)} = \left\| \delta_{ii} - \sum_{\vec{k}} Q_i(\vec{k}) Q_{i'}(\vec{k}) \right\|,$$

(3, 2; 13)

where i and i'are indices running 1,2,...,n. (See Appendix (A1,2) for justification of the last step.) Thus

$$\Gamma(z) = \left\| \delta_{ii} - \frac{1}{V} \sum_{\vec{k}} \frac{F_i(\vec{k}) F_i(\vec{k})}{z - \omega(\vec{k})} \right\|.$$
(3,2;14)

Using (3,1;2), one may write

$$\sum_{\vec{k}} \frac{\overline{F_{\ell}(\vec{k})} F_{\ell'}(\vec{k})}{z - \omega(\vec{k})} \longrightarrow \frac{1}{8\pi^{3}} \int d^{3}\vec{k} \frac{\overline{F_{\ell}(\vec{k})} F_{\ell'}(\vec{k})}{z - \omega(\vec{k})} \equiv I_{\ell\ell'}.$$
(4,2;15)

Hence, $\Gamma(z)$ is a sum of a finite number of terms; one being unity, others being products of up to N intergals of the type I_{iji} , the integrands of which involve only known functions.

Since G'(z)Log $\Gamma(z)$ is analytic above and below the real axis and on the real axis between 0 and w_0 , the path P may be allowed to approach the locus L. Let $z = x + i\epsilon$. Then, (3,2;12) becomes

$$g = \lim_{\epsilon \to 0} \left\{ -\frac{1}{2\pi i} \left[-\int_{w_{\bullet}}^{\infty} dx G'(x+i\epsilon) dog \Gamma(x+i\epsilon) + \int_{w_{\bullet}}^{\infty} dx G'(x-i\epsilon) dog \Gamma(x-i\epsilon) \right] \right\}$$

(3,2)

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or

$$Q = \frac{1}{2\pi i} \left\{ \int_{\omega_0}^{\infty} dx G'(x) \left[\lim_{\epsilon \to 0} \left(\partial \log \Gamma(x+i\epsilon) - \partial \log \Gamma(x-i\epsilon) \right) \right] \right\}.$$
(3,2;16)

Let $\Gamma(x + i\varepsilon) = u(x) + iv(x)$. From (3,2;14), it then follows that $\Gamma(x - i\varepsilon) = u(x) - iv(x)$. By defining

$$\lim_{\epsilon \to 0} \left| \Gamma(x \pm i \epsilon) \right| = M(x)$$

and

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$$\lim_{\epsilon \to 0} \operatorname{arg} \Gamma(x \pm i\epsilon) = \pm H(x),$$

(3,2;17)

one may write

$$\lim_{\epsilon \to 0} \left\{ \log \Gamma(x+i\epsilon) - \log \Gamma(x-i\epsilon) \right\}^{2} = 2i \bigoplus (x) .$$

Hence, from (3,2;16), one concludes that

$$g = \frac{1}{TT} \int_{\omega_0}^{\infty} dx G'(x) \oplus (x),$$

(3,2;18)

where, in summary, from (3,2;11), (3,2,13), (3,2;14), (3,2;15), and (3,2;17), one has

$$\begin{aligned} & (\mathbf{x}) = \lim_{\epsilon \to 0} \operatorname{Qrg} \Gamma(\mathbf{x} + i\epsilon) \\ & \Gamma(\mathbf{x} + i\epsilon) = \left\| \delta_{1i'} - \frac{1}{8\pi^3} \int \frac{F_i(\vec{k}) F_{i'}(\vec{k})}{\mathbf{x} - \omega(\vec{k}) + i\epsilon} d^3\vec{k} \right\| \\ & -\pi < \operatorname{Qrg} \Gamma \leq +\pi \\ & i = 1, 2, \cdots, n \\ & i' = 1, 2, \cdots, n. \end{aligned}$$

$$(3, 2; 19)$$

This result makes it possible to perform sums over solutions of a multidimensional secular equation without directly evaluating the density of the solutions, in the limit as the dimensionality of the secular equation becomes infinite.

(3,3) A Separable Potential Model in Particle Field Theory

In the following, the procedures developed previously are applied to the investigation of a two-body separable potential, field-theoretic model. This model is of interest because it is an exactly soluble model and is useful for testing calculational techniques. Previous studies of this model have been made by Urrechaga-Altuna and Childress,⁶ Henley and Thirring,⁷ Kazes,⁸ Yamaguchi,⁹ and Yamguchi and Yamaguchi¹⁰ to mention but a few. 27

(3,2)

(3,3)

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Consider the simple separable potential model in which light neutral scalar bosons of rest mass, m_0 , interact with a static heavy neutral boson of mass M in a manner described by the Hamiltonian,

 $H = H'_{2} + H''_{2}$

where

$$H_{2}' = \hbar \sum_{\vec{k}} \omega(k) b_{\vec{k}}^{\dagger} b_{\vec{k}},$$

(3,3;2)

$$H''_{z} = \lambda \hbar \sum_{\vec{k} \cdot \vec{k}} f(k) f(\vec{k}) b_{\vec{k}}^{\dagger} b_{\vec{k}'}$$

(3,3;3)

$$\hbar \omega(k) = C (k^2 + \mu^2)^{1/2},$$

(3,3;4)

 λ is the interaction coupling constant, c is the speed of light and $\mu = m_o c/h$. The function f(k) is a function of the magnitude of the wave vector \vec{k} and is assumed to have such analytic properties as may be necessary to guarantee the existence of any integrals encountered. The operators $b_{\vec{k}}^{\dagger}$ and $b_{\vec{k}}$ respectively designate creation and annihilation operators for light bosons of momentum h \vec{k} and satisfy the

(3,3;1)

(3,3)

commutation relations

$$\begin{bmatrix} b_{\vec{k}}, b_{\vec{k}'}^{\dagger} \end{bmatrix} = \delta_{\vec{k} \cdot \vec{k}'}$$
$$\begin{bmatrix} b_{\vec{k}}, b_{\vec{k}'} \end{bmatrix} = 0$$

For notational convenience the natural system of units

$$h = c = 1$$
 (3,3;5)

will be used in the following,

It may be noted that (3,3;1) is of the form of (2,4;1) through (2,4;3) wherein the following identifications are made;

$$a_{j} \rightarrow b_{\vec{k}}$$

$$\alpha_{jj'} = \beta_{jj'} = \eta_{j} = h_{\circ} = 0$$

$$\delta_{jj'} \rightarrow \delta_{\vec{k}\vec{k}'} = 2 \left[\omega(k) \delta_{\vec{k}\vec{k}'} + \lambda f(k) f(k) \right]$$
(3,3;6)

Hence, it follows from the procedure outlined in (2,4) that, if γ is positive definite, there exists a canonical transformation, which reduces (3,3;1) to the form

$$H = \sum_{\nu} \Omega_{\nu} B_{\nu}^{\dagger} B_{\nu}$$

(3,3;7)
with

$$[B_{\nu}, B_{\nu}^{\dagger}] = \delta_{\nu \nu},$$

 $[B_{\nu}, B_{\nu}] = 0.$

In these equations v and v' are members of an index set whose elements may be put into one-to-one correspondence with the domain of \vec{k} , (3,1;1), $\Omega_v = \sqrt{\Omega_v^2}$, and the Ω_v^2 's are the solutions for Ω^2 of the secular equation (2,4;9); i.e.,

$$\|\Omega^2 \delta_{\vec{k}\vec{k}'} - \frac{1}{4} \sum_{\vec{k}''} \delta_{\vec{k}''\vec{k}'} \| = 0,$$

or

$$O = \left\| \sum_{\vec{k}''} \left[\Omega^2 \delta_{\vec{k}\vec{k}''} \delta_{\vec{k}''\vec{k}} - \frac{1}{4} \delta_{\vec{k}\vec{k}''} \delta_{\vec{k}''\vec{k}} \right\| \right\|$$

$$= \left\| \sum_{\vec{k}''} \left[\Omega^{2} \delta_{\vec{k}'\vec{k}'} \delta_{\vec{k}''\vec{k}'} - \frac{1}{2} \Omega \delta_{\vec{k},\vec{k}''} \delta_{\vec{k}''\vec{k}'} \right] \right\| \\ + \frac{1}{2} \Omega \delta_{\vec{k}''\vec{k}'} \delta_{\vec{k}''\vec{k}} - \frac{1}{4} \delta_{\vec{k}\vec{k}''} \delta_{\vec{k}''\vec{k}'} \right] \right\|$$

$$= \left\| \sum_{\vec{k}''} \left\{ \left[\Omega S_{\vec{k}\vec{k}''} - \frac{1}{2} \delta_{\vec{k}\vec{k}''} \right] \left[\Omega S_{\vec{k}''\vec{k}'} + \frac{1}{2} \delta_{\vec{k}''\vec{k}'} \right] \right\} \right\|.$$

$$\|\Omega S_{\vec{k}\vec{k}} - \frac{1}{2} \delta_{\vec{k}\vec{k}} \| \cdot \|\Omega S_{\vec{k}\vec{k}} + \frac{1}{2} \delta_{\vec{k}\vec{k}} \| = 0.$$

$$(3.3:8)$$

Note that the solutions obtained by setting either one of the immediately preceding determinants equal to zero are just the negatives of the solutions got by setting the other to zero. Hence, all the $\Omega_v^{2_1}$ s may be obtained by solving the secular equation for either determinant. However, equation (3,3;8) is valid only for γ positive definite; and one way to determine the positive definite character of γ is to find its eigenvalues. Hence, if the solutions to

$$\|\Omega \delta_{\vec{k}\vec{k}} - \frac{1}{2}\delta_{\vec{k}\vec{k}}\| = 0$$

are positive, then γ is positive definite and the solutions are the required ones; otherwise the system fails to have a ground state. Substituting (3,3;6) into this secular equation yields

$$\left\| \left(\Omega - \omega(\mathbf{k}) \right) \delta_{\vec{k}\vec{k}'} - \lambda f(\mathbf{k}) f(\mathbf{k}') \right\| = \prod \left(\Omega - \Omega_{\mathbf{k}} \right)^{2} O.$$
(3,3;9)

To solve this equation, first regard the normalization volume, V, as finite and consider the function D(z) of a complex variable, z, defined by

$$D(z) = \frac{\prod (z - \Omega_{y})}{\prod (z - \omega(k))}.$$
(3.3:10)

(3,3)

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$$D(z) = \frac{1}{\prod_{k} (z - \omega(k))} \left\| (\Omega - \omega(k)) \delta_{\vec{k}\vec{k}'} - \lambda f(k) f(k') \right\|$$

$$(3,3;11)$$

$$= \left\| \delta_{\vec{k}\vec{k}'} - \frac{\lambda f(k)f(k')}{[z - \omega(k')]} \right\|$$

$$(3.3; 12)$$

$$= | - \lambda \sum_{\vec{k}} \frac{f^{2}(k)}{\vec{z} - \omega(k)} \cdot$$
(3,3;13)

In the last step, use is made of the theorem proved in Appendix (A1,2). By inspection of (3,3;10), the values of the Ω_v 's are characterized as all values of z for which D(z) vanishes together with the set of all values of $\omega(k)$ except perhaps for those values of $\omega(k)$ such that $D(z) = \infty$.

To investigate the character of D(z) in the limit $V \rightarrow \infty$, regard z as fixed at any value remaining different from any of the (discrete) values of $\omega(k)$ as the limit $V \rightarrow \infty$ is taken so that the sum in (3,3;13) remains well defined. Then, in view of (3,1;2), equation (3,3;13) approaches

$$D(z) = \left[-\frac{\lambda V}{8\pi^3} PP \int d^3 \vec{k} \frac{f^2(k)}{z - \omega(k)} \right]$$

(3,3)

$$D(z) = \left| -\frac{\lambda V}{4\pi^2} PP \int_{-\infty}^{+\infty} \frac{k^2 f^2(k)}{z - \omega(k)}, \frac{k^2 f^2(k)}{z - \omega(k)} \right|^{-\infty}$$
(3.3:14)

where PP stands for "principal part". In the limit $V \rightarrow \infty$, the set of all values of $\omega(k)$ becomes the continuum of real values $\geq \mu$. For sufficiently well behaved functions f(k), the integral in (3,3;14) will remain finite for $z \geq \mu$ in which case the solutions to (3,3;9) will be all (real) values $\geq \mu$ together with the solutions for z of the equation D(z) = 0.

Suppose, for the sake of a more detailed discussion of a specific problem, that f(k) is defined in the following way:

$$k^{2}f^{2}(k) = \frac{4\pi^{2}}{V(k^{2}+\mu^{2})}$$

(3,3;15)

Substitution of (3,3;15), (3,3;4), and (3,3;5) into (3,3;14) yields

$$D(z) = | + \lambda I(z),$$

(3,3;16)

where

..

$$I(z) = PP \int_{-\infty}^{+\infty} \varphi_{z}(k) dk$$

(3,3;17)

-33

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$$f_{z}(k) = \frac{1}{(k^{2} + \mu^{2})(1k^{2} + \mu^{2} - z)}$$

(3,3;18)

Evaluation of (3,3;17) as a function of z yields



(See Appendix (A2,1) for the details of this evaluation.)

The analytical form of (3,3;17), (3,3;18), and (3,3;19) leads to the qualitative plot of I(z) versus z shown in the following diagram.

and



From (3,3;16) and the above plot of I(z), it follows that D(z) has no infinities for $z \ge \mu$. Hence, the set of single particle energy levels, $[\Omega_{\nu}]_{\nu}$, contains the set, $[\omega(k)]_{\vec{k}}$, all the elements of which are positive. For a given value of λ all other elements of $[\Omega_{\nu}]_{\nu}$ are given by the values of z for which $-1/\lambda = I(z)$. If the values of z obtained by setting $-1/\lambda$ equal to I(z) and solving for z are positive, then γ is positive definite. If any of the values of z so obtained are nonpositive, then γ is not positive definite, contrary to the requirement for the validity of the procedures used to obtain the secular equation, (3,3;9), and to the original requirement that the system possess a ground state. Thus, any values of λ .

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which lead to a nonpositive element of $[\Omega_v]_v$ will be excluded from further consideration.

Consider the following four ranges of the coupling constant, λ .

1. $-1/\lambda < -(\pi-2)/\mu^2$. For λ in this range there is no value of z for which D(z) = 0. For lack of physically interesting results, this case will be given no further consideration.

2. $-(\pi - 2)/\mu^2 \le -1/\lambda < 0$. For λ in this range there is a positive, unique value of z for which D(z) = 0. Denote that value of z by Ω_{vx} . Note: $\Omega_{vx} \ge \mu$.

3. $0 \leq -1/\lambda \leq 2/\mu^2$. For λ is this range there is a nonpositive, unique value of z such that D(z) = 0. This case is of no further interest on the basis of the discussion in the previous paragraph.

4. $2/\mu^2 < -1/\lambda$. For λ in this range there is a positive, unique value of z for which D(z) = 0. Denote that value of z by $\Omega_{\sqrt{0}}$ ($0 < \Omega_{\sqrt{0}} < \mu$).

For the two cases of interest; namely, case 2 and case 4, it follows that

$$\left[\Omega_{\nu}\right]_{\nu} = \left[\Omega_{\nu^{*}}\right] \cup \left[\omega(k)\right]_{\vec{k}}$$

and

$$\left[\Omega_{\gamma}\right]_{\gamma} = \left[\Omega_{\gamma}\right] \cup \left[\omega(k)\right]_{\vec{k}}$$

respectively.

These results may be given the following interpretation: in the presents of interaction, the light bosons behave like a collection

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of noninteracting particles, or "quasi-particles". The ground state of the system is the vacuum state $|0\rangle$, characterized by $B_v|0\rangle \equiv |0\rangle$, with zero energy eigenvalue. If $-1/\lambda > 2/\mu^2$, then the first excited state is the single quasi-particle state $B_v^{\dagger}o|0\rangle$ with energy $\ln \Omega_v o$. This state would be relatively stable against external perturbative influences because of separation in energy of this state from other eigenstates of the system. The other single quasi-particle states have the continuous band of energy values $\geq \mu$. If $-(\frac{\pi-2}{2}) \leq -\frac{1}{\lambda} < 0$, the situation is similar except that in place of $B_v^{\dagger}o|0\rangle$, one has instead the state $B_v^{\dagger}w|0\rangle$ whose energy is embeded in the continuum band. Such a quasi-particle state would be unstable.

(3,4) The Polaron Problem

In this section both the procedures of Chapter 2 and the calculational technique of section (3,2) will be employed in an investigation of the ground state energy of the polaron.

The polaron problem originates from studies in solid state physics. Its intrinsic values, then, make this problem worthy of considerable interest. This interest is enhanced by the fact that the polaron is a relatively simple, yet realistic example of a large class of many body problems in various areas of physics. Hence, the polaron problem may be used as a tool to test approximation methods which may be applied to more complicated problems.

The polaron problem consists of a nonrelativistic quantum mechanical description of a single conduction electron within an ionic crystal such as NaCl. The entity consisting of the conduction electron with crystal mass, m, and its self-induced polarization field is called the polaron.

The Hamiltonian for the polaron was derived by Fröhlich and may be expressed in the language of second quantization as²

$$H(\vec{K}) = \left(\vec{K} - \sum_{\vec{k}} \vec{k} a_{\vec{k}}^{\dagger} a_{\vec{k}}\right)^{2} + \sum_{\vec{k}} a_{\vec{k}}^{\dagger} a_{\vec{k}}$$

+ $i \delta_{o} \sum_{\vec{k}} \frac{1}{k} (a_{\vec{k}}^{\dagger} - a_{\vec{k}}),$
(3,4;1)

where H is written in terms of dimensionless variables, and

$$\delta_{o} = \sqrt{\frac{4\pi\alpha}{S}}$$
(3,4;2)

where α is the polaron coupling constant and S is the dimensionless normalization volume. In (3,4;1), \vec{K} is the total wave vector of the system and is a constant of the motion. The index, \vec{k} , takes on the quantized values of the wave vectors of the polarization field quanta, as given by (3,1;1).

The term

$$\sum_{\vec{k}} a^{\dagger}_{\vec{k}} a_{\vec{k}}$$

represents the energy of the polarization field in the absence of interaction with the conduction electron, and the operators $a_{\vec{k}}$ and $a_{\vec{k}}^{\dagger}$ satisfy the usual commutation rules,

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(3,4)

$$\left[a_{\vec{k}}, a_{\vec{k}}^{\dagger}\right] = \delta_{\vec{k}\vec{k}}.$$

and

$$[a_{\vec{k}}, a_{\vec{k}}] = 0.$$

The operator

 $\sum_{\vec{k}} \vec{k} a^{\dagger}_{\vec{k}} a_{\vec{k}}$

represents the total wave vector of the polarization field.

The term

$$\left[\overline{K} - \sum_{\vec{k}} \overline{k} a_{\vec{k}}^{\dagger} a_{\vec{k}}\right]^{2}$$

represents the kinetic energy of the conduction electron expressed in terms of polarization field quantities.

The term

$$i \delta_{o} \sum_{\vec{k}} \frac{1}{k} (a_{\vec{k}}^{\dagger} - a_{\vec{k}})$$

represents the potential energy of interaction of the polarization field with the electron.

Note that if $\vec{K} = \vec{0}$ in (3,4;1), then this expression becomes the Hamiltonian for a polaron at rest, i.e.

$$H = \left(\sum_{\vec{k}} \vec{k} a_{\vec{k}}^{\dagger} a_{\vec{k}}\right)^{2} + \sum_{\vec{k}} a_{\vec{k}}^{\dagger} a_{\vec{k}}$$
$$+ i \delta_{o} \sum_{\vec{k}} \frac{1}{k} \left(a_{\vec{k}}^{\dagger} - a_{\vec{k}}\right).$$

The ground state energy of a polaron at rest (in other words, the self-energy of the polaron) is just the least eigenvalue, E_0 , of (3,4;3). Any eigenvalue of (3,4;3) is clearly a function of the polaron coupling constant, α . In order to maintain a greater degree of generality, α will be regarded as an arbitrary positive parameter, and E_0 will be expressed as a function of α .

A great deal of work has been done to evaluate the self-energy of the polaron. As a result, the dependence of E_0 upon α is fairly well known. It is advantageous, then, to review the research which bears directly on the development of the approach to be taken here.

In the case of weak coupling, i.e. $\alpha \rightarrow 0$, it is possible to treat the interaction term,

$$i\delta_{o}\sum_{\vec{k}}\frac{1}{k}(a_{\vec{k}}^{\dagger}-a_{\vec{k}}),$$

as a perturbation² of the remainder of the Hamiltonian, (3,4;3). The result of this treatment may be expressed as 40

(3,4)

(3,4;3)

$$E_{o}^{\text{pert.}} = -\alpha - 0.0160\alpha^{2} + O(\alpha^{3}).$$
(3,4;4)

In this approximation the second order correction, -0.0160 α^2 , is less than 2% of the first order term, - α , at α = 1, and is less than . 10% of the first order term at α = 6.

A weak coupling variational method^{2,11,12,13,14} has been developed for evaluating E_0 as a function of α . Basically, this method may be outlined in the following manner.

First, define a transformation, such as (2,1;11), designed to eliminate linear terms in H, (3,4;3). Let

$$a_{\vec{k}} = b_{\vec{k}} + i f_{\vec{k}}$$

$$a_{\vec{k}}^{\dagger} = b_{\vec{k}}^{\dagger} - i f_{\vec{k}}^{*}.$$
(3,4;5)

Substituting (3,4;5) into (3,4;3), one obtains the following expression:

$$H = H_0 + H_1 + H_2 + H_3 + H_4,$$
(3,4;6)

where

$$H_{o} = \sum_{\vec{k}} \left\{ \omega(k) f_{\vec{k}} f_{\vec{k}}^{*} - \frac{\lambda_{o}}{k} \left(f_{\vec{k}} + f_{\vec{k}}^{*} \right) \right\} + \vec{u} \cdot \vec{u}, \qquad (3,4;7)$$

$$\begin{split} H_{i} &= i \sum_{\vec{k}} \left\{ \left[\frac{\delta}{k} - f_{\vec{k}} \,\omega(k) \right] b_{\vec{k}}^{\dagger} - \left[\frac{\delta}{k} - f_{\vec{k}}^{\ast} \,\omega(k) \right] b_{\vec{k}} \right\} \\ &+ 2i \,\vec{u} \cdot \sum_{\vec{k}} \vec{k} \left(f_{\vec{k}}^{\ast} b_{\vec{k}} - f_{\vec{k}} \,b_{\vec{k}}^{\dagger} \right), \\ H_{2} &= \sum_{\vec{k}} \omega(k) b_{\vec{k}}^{\dagger} b_{\vec{k}} + 2 \,\vec{u} \cdot \sum_{\vec{k}} \vec{k} \,b_{\vec{k}}^{\dagger} b_{\vec{k}} \\ &- \sum_{\vec{k}} \left\{ (\vec{k} \cdot \vec{k}) \left[f_{\vec{k}} f_{\vec{k}} \cdot b_{\vec{k}}^{\dagger} b_{\vec{k}} - 2 f_{\vec{k}} f_{\vec{k}}^{\ast} \cdot b_{\vec{k}} b_{\vec{k}} + f_{\vec{k}}^{\ast} f_{\vec{k}}^{\ast} b_{\vec{k}} b_{\vec{k}} \right] \right\}, \\ &\qquad (3,4;8) \end{split}$$

$$H_{3} = 2 i \sum_{\vec{k},\vec{k}'} \left\{ (\vec{k} \cdot \vec{k}') \left[f_{\vec{k}'}^{*} b_{\vec{k}}^{\dagger} b_{\vec{k}} b_{\vec{k}'} - f_{\vec{k}} b_{\vec{k}}^{\dagger} b_{\vec{k}'} b_{\vec{k}'} \right] \right\},$$
(3,4;10)

$$H_{4} = \sum_{\vec{k} \cdot \vec{k}'} (\vec{k} \cdot \vec{k}') b_{\vec{k}}^{\dagger} b_{\vec{k}'}^{\dagger} b_{\vec{k}} b_{\vec{k}'}$$

(3,4;11)

(3,4)

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(3,4)

(3,4;12)

$$\omega(k) = |+k^2$$

and

$$\vec{u} = \sum_{\vec{k}} \vec{k} f_{\vec{k}} f_{\vec{k}}^{*}.$$

(3,4;13)

In the complete reduction scheme of Chapter 2, one would now set the coefficients of $b_{\vec{k}}^{\dagger}$ and $b_{\vec{k}}$ in (3,4;8) to zero, and thus define the function, $f_{\vec{k}}$. However, in the weak coupling variational approach, $f_{\vec{k}}$ is left unspecified at this point. The next step is to construct a weak coupling trial ground state, vector, $|w.c.\rangle$. Then the ground state expection value of H in (3,4;6) is calculated with respect to this state, $|w.c.\rangle$. Finally, the expectation value of H is minimized with respect to the function, $f_{\vec{k}}$, to obtain the variationally optimal choice for $f_{\vec{k}}$.

Suppose that one takes as a trial ground state $|w.c.\rangle = |0\rangle$, the (normalized) state defined by

$$b_{\vec{k}} | 0 \rangle \equiv 0. \tag{3.4.14}$$

This approximation amounts to optimally accounting for the terms of the interaction Hamiltonian which are linear in creation and destruction operators, but neglects the quadratic and higher order interaction terms generated in the elemination of the linear terms. This neglect is of order α^2 , in an expansion of E_o about $\alpha = 0$. In this case one obtains the following results for the expectation value of H:

$$\langle w.c. | H | w.c. \rangle = \langle 0 | H | 0 \rangle = H_{o}.$$

(3,4;15)

Hence, the weak coupling variational approximation to the ground state energy, $E_0^{W.C.}$, of the polaron at rest is given by (3,4;7), (3,4;12), and (3,4;13) as

$$E_{o}^{\text{w.c.}} = \sum_{\vec{k}} \left\{ (1+k^{2})f_{\vec{k}}f_{\vec{k}}^{*} - \frac{\delta_{e}}{k}(f_{\vec{k}} + f_{\vec{k}}^{*}) \right\} + \left[\sum_{\vec{k}} \vec{k} f_{\vec{k}}f_{\vec{k}}^{*} \right]^{2}$$
(3,4;16)

Minimization of $E_0^{w.c.}$ with respect to $f_{\vec{k}}$ and $f_{\vec{k}}^*$ yields

$$f_{\vec{k}} = f_{\vec{k}}^* = \frac{\delta_0}{k} \left(\frac{1}{1 + 2\vec{u} \cdot \vec{k} + \vec{k}} \right).$$

(3,4;17)

If one substitutes (3,4;17) into (3,4;13), one obtains the result that $\vec{u} = \vec{0}$. Hence, the expression for $f_{\vec{k}}$ becomes

$$f_{\vec{k}} = \frac{\delta_o}{k} \left(\frac{1}{1+k^2} \right),$$

(3,4;18)

(3,4)

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Substitution of (3,4;18) into (3,4;16) for $E_0^{W,C}$ gives

$$E_{o}^{w.c.} = -y_{o}^{n^{2}} \sum_{\vec{k}} \frac{1}{\vec{k}^{2}(1+\vec{k}^{2})} \cdot$$

(3,4;19)

Replacing γ_0 in (3,4;19) by the expression in (3,4;2) and performing the integration resulting from the substitution,

$$\sum_{\vec{k}} \xrightarrow{S \to \infty} \frac{S}{8\pi^3} \int d^3 \vec{k} ,$$

one obtains

$$E_{o}^{w.c.} = -\alpha$$
.

(3,4;20)

One may now consider an improvement on the weak coupling variational method suggested by E. P. Gross¹⁵. Initially, one makes a transformation, such as (3,4;5), on (3,4;3), leaving the function $f_{\vec{k}}$ unspecified. Next, a canonical transformation designed to reduce the quadratic part, H₂, of (3,4;6) is made. Finally, the expectation value of H with respect to the least energy eigenstate of H₂ is calculated, and the result is minimized with respect to the $f_{\vec{k}}$'s. The resulting equation obtained for determining $f_{\vec{k}}$ is too complicated for practical use. Instead a specific functional form is chosen for $f_{\vec{k}}$ involving variational parameters for the function, $f_{\vec{k}}$. One then minimizes with respect to these parameters in the final analysis.

Following the procedure outlined in the previous paragraph, one makes a transformation of the form of (3,4;5) on H, (3,4;3) where it is assumed that

$$f_{\bar{k}} = f_{k} = f_{k}^{*} = \frac{\delta_{o}}{k} \left(\frac{\lambda k_{o}^{2}}{k^{2} + k_{o}^{2}} \right),$$

(3,4;21)

with λ and k_0 to be treated as variational parameters. In this case H may be written as

$$-1 = H_0 + H_1 + H_2 + H_3 + H_4$$
,

(3,4;22)

where

$$H_{o} = \sum_{\vec{k}} \left\{ \omega(k) f_{k}^{2} + \frac{2\delta_{o}}{k} f_{k} \right\},$$

(3,4;23)

(3,4)

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(3,4)

$$H_{1} = i \sum_{\vec{k}} \left\{ \left[\omega(k) f_{k} - \frac{y_{0}}{k} \right] (b_{\vec{k}} - b_{\vec{k}}^{\dagger}) \right\},$$

$$H_{2} = \sum_{\vec{k}} \omega(k) b_{\vec{k}}^{\dagger} b_{\vec{k}} + \sum_{\vec{k}, \vec{k}'} \left\{ (\vec{k} \cdot \vec{k}') \cdot \frac{1}{k} f_{\vec{k}'} (b_{\vec{k}}^{\dagger} b_{\vec{k}'}^{\dagger} + b_{\vec{k}} b_{\vec{k}'}) + 2 f_{k} f_{k'} b_{\vec{k}}^{\dagger} b_{\vec{k}'} \right\},$$

$$(3.4:25)$$

$$H_{3} = 2i \sum_{\vec{k},\vec{k}} \left\{ (\vec{k} \cdot \vec{k}) \left[f_{\vec{k}} b_{\vec{k}} b_{\vec{k}} b_{\vec{k}} b_{\vec{k}'} + f_{\vec{k}} b_{\vec{k}}^{\dagger} b_{\vec{k}'} \right] \right\},$$

(3,4;26)

$$H_{4} = \sum_{\vec{k},\vec{k}'} (\vec{k}\cdot\vec{k}) b_{\vec{k}}^{\dagger} b_{\vec{k}'}^{\dagger} b_{\vec{k}} b_{\vec{k}'},$$

(3,4;27)

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and w(k) is given by (3,4;12).

Now H_2 , (3,4;25), may be put into the form of (2,4;1) by making the following replacements:



Using (3,4;28), (3,4;21), and the fact that α is positive, one may observe that u and v as given in (2,4;11) are both positive definite. Hence, the procedures developed in Chapter 2 are valid for the reduction of H₂.

Thus, there exists a canonical transformation that completely reduces H_2 to the form of (2,4;7). This transformation may be written as

(3,4;29)

 $b_{k} = \sum_{\nu} \phi_{k,\nu} \left[\alpha_{k,\nu} B_{\nu} + \beta_{k,\nu} B_{\nu}^{\dagger} \right]$

where $[\varphi_{\vec{k}}, v]_v$ is a complete orthonormal set of functions of \vec{k} , orthonormal in the sense that $\sum_{k} \varphi_{k,v} \varphi_{k,v'} = \delta_{vv'}$, and $\alpha_{k,v}$ and $\beta_{\vec{k},\nu}$ are given by

$$\mathcal{Q}_{\vec{k},\nu} = \frac{\Omega_{\nu} + \omega(k)}{2 \sqrt{\Omega_{\nu} \omega(k)}}, \quad \beta_{\vec{k},\nu} = \frac{\Omega_{\nu} - \omega(k)}{2 \sqrt{\Omega_{\nu} \omega(k)}},$$

where $[\Omega_{v}]_{v}$ and the $\varphi_{\vec{k},v}$'s are chosen to reduce H₂. Substitution of (3,4;29) and 3,4;28) into H yields

$$H = H_0' + H_2' + H_1' + H_3' + H_4' + H_2',$$

(3,4;30)

where

$$H_{o}' = \sum_{k} \left[\omega(k) f_{k}^{2} - \frac{2N}{k} f_{k} \right] + \frac{1}{2} \sum_{v} \Omega_{v}$$
$$- \sum_{k} \frac{1}{2} \left[\omega(k) + 2k^{2} f_{k}^{2} \right],$$

(3,4;31)

(3,4)

(3,4)

$$H_{z}' = \sum_{\mu} \Omega_{\mu} B_{\mu}^{\dagger} B_{\mu}$$

(3,4;32)

 H_2'' is a quadratic term that results from substituting (3,4;29) into H_4^- , H_1' , H_3' , and H_4' are linear, cubic, and quartic, respectively, in B_V and B_V^+ , $\Omega_V = \pm 1 \Omega_V^2$, and the Ω_V^2 's are the solutions for Ω^2 to secular equation, (2,4;9), with (2,4;11) and (3,4;28):

$$D = \left\| \left(\Omega^{2} - \omega^{2}(k) \right) \delta_{\vec{k}\vec{k}'} - 4 \omega(\vec{k}) \left[\vec{k} \cdot \vec{k} \right] f_{\vec{k}} f_{\vec{k}} \right\|$$
$$= \left\| \left(\Omega^{2} - \omega^{2}(k) \right) \delta_{\vec{k}\vec{k}'} - 4 \omega(\vec{k}) \left[\vec{k} \cdot \vec{k} \right] f_{\vec{k}} f_{\vec{k}} \right\| \cdot \left\| \frac{\omega(\vec{k})}{\omega(\vec{k})} \right\|.$$

Therefore,

$$\left\| \left(\Omega^2 - \omega^2(k) \right) \delta_{\vec{k}\cdot\vec{k}} - 4 \int \omega(k) \omega(\vec{k}) \left(\vec{k}\cdot\vec{k} \right) f_k f_{\vec{k}} \right\| = 0.$$

(3,4;33)

(3, 4; 34)

One may take as a trial ground state of the system the exact ground state of H_2^1 , i.e., the state, $| 0 \rangle$, such that

 $B_{\nu}|o\rangle \equiv 0.$

Using the completeness of the set $[\varphi_{\vec{k},\nu}]_{\nu}$ and symmetry arguments, one may show ^{12,15} that

 $\langle 0|H'_{1} + H'_{2} + H'_{3} + H'_{4} + H''_{2}|0\rangle = 0.$

(3,4;35)

Hence, the ground state energy of a polaron at rest, E_0 , may be approximated by

 $E_{\circ} = \langle 0|H|0 \rangle = H'_{\circ}$.

(3,4;36)

; (3,4;37)

Substitution of (3,4;31), (3,4;28), and (3,4;12) into (3,4;36) yields

$$E_o = g_o + g_2 ,$$

where

$$g_o = \sum_{k} \left[f_k^2 - \frac{2\aleph_o}{k} f_k \right]$$

(3,4;38)

(3,4)

and

$$g_{z} = \frac{1}{2} \left\{ \sum_{y} \Omega_{y} - \sum_{\overline{k}} \omega(k) \right\}.$$
(3,4;39)

To evaluate (3,4;38), one uses (3,4;21), (3,4;2), and the replacement

$$\sum_{\vec{k}} \xrightarrow{S \to \infty} \frac{S}{8\pi^3} \int d^3 \vec{k} ,$$

integrating first over angles and then, by the method of residues, over the magnitude of \vec{k} , to obtain

$$g_o = -\alpha k_o \left[2\lambda - \frac{\lambda^2}{2} \right].$$

(3,4;40)

The expression for g_2 , (3,4;39), may be evaluated by the procedure described in section (3,2). (See Appendix (A2,2).) The result of this evaluation is

$$g_2 = \frac{3}{\pi} \int_{0}^{\infty} dw w (H)(w),$$

(3,4;41)

where

$$(H)(w) = \operatorname{arg} \left[X(w) + i Y(w) \right],$$

(3,4;42)

$$X(w) = \left| + \frac{2\alpha k_0^3 \lambda^2}{3} \left\{ \frac{4k_0^2 (1-k_0^2)^2 + (3k_0^2 - 1)(w^2 + 2 - k_0^2)(w^2 + k_0^2) - k_0 (w^2 + k_0^2)^2}{(w^2 + 2 - k_0^2)^2 (w^2 + k_0^2)^2} \right\}_{\eta}$$

(3,4;43)

and

$$Y(w) = \frac{2\alpha k_{o}^{4} \lambda^{2}}{3} \left\{ \frac{w}{(w^{2} + k_{o}^{2})^{2}} \right\},$$

(3,4;44)

Expansion of g_2 in the weak coupling limit, $\alpha \rightarrow 0$, and evaluation of the resulting integrals to first order in α yields

$$g_2 = \frac{\alpha k_o^3 l^2}{2} \cdot$$

(3,4;45)

: X

(See Appendix (A2,3).)

If one now substitutes (3,4;45) and (3,4;40) into the approximation for the ground state energy of a polaron at rest, (3,4;36), he obtains, to first order in α ,

$$E_{o} = -\alpha k_{o} \left[2\lambda - \frac{\lambda^{2}}{2} \right] + \frac{1}{2} \alpha k_{o}^{3} \lambda^{2} + O(\alpha^{2}).$$
(3.4:46)

Minimizing E with respect to k_{0} and $\lambda,$ one finds that the optimum choice for k_{0} and λ is

$$k_{o} = \lambda = 1.$$

(3,4;47)

Hence, (3,4;46) becomes

$$E_{o} = -\alpha + O(\alpha^{2}). \qquad (3,4;48)$$

Thus, to first order in the coupling constant, α , the approximation for E_o given by (3,4;37) is exactly equal to the Lee-Low-Pines weak coupling result, E_o^{w.c.}.

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One may evaluate E_0 in (3,4;37) to second order in α and obtain the result,

$$E_{o} = -\alpha - 0.0126\alpha^{2} + O(\alpha^{3}).$$

(3,4;49)

(See Appendix (A2,3).)

This result compares favorably with the second order result, (3,4;4), given by perturbation theory, the coefficient of the second order term in the former being approximately 80% of that of the latter.

Hence, the result of this approximation in the weak coupling limit is superior to the Lee-Low-Pines weak coupling result and slightly inferior to the perturbation theory result. However, it has the distinct advantage over the perturbation approximation that it is variationally correct for all values of α ; i.e., the exact self-energy of the polaron is less than or equal to the result of this approximation.

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(3.4)

CHAPTER 4

CONCLUSION

It is shown that the quadratic Hamiltonian for a broad class of systems may be reduced to the form of the Hamiltonian for a collection of noninteracting bosons by means of a succession of canonical linear transformations. The reduction procedure leads to a single secular equation, the solutions of which determine the eigenvalues of the Hamiltonian. The application of the procedure is illustrated by two problems of physical interest; namely, a simple separable potential model from particle field theory and the polaron problem of solid state physics. In this way the primary and secondary objectives of this research are accomplished. It remains to attain the final objective, to indicate a method of employing the procedure herein developed to systems whose Hamiltonians may be approximated by quadratic ones of the class treated.

Consider such a system, and denote the exact and quadratic, approximate Hamiltonians by H and H₂, respectively. H₂ may or may not be the quadratic part of H, depending on the specific physical system of interest.

A variational approximation to a given eigenvalue of H may be obtained in the following way. Examine H_2 to determine the form of the canonical transformation which would reduce it in the light

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of the procedure developed. However, instead of determining the matrix elements of this transformation to reduce H_2 , apply the transformation to H, leaving these matrix elements unspecified. Calculate the expectation value of H with respect to the appropriate eigenstate of H_2 in its reduced form and minimize the result with respect to the matrix elements of the transformation. In this way one may obtain variationally correct results for the expectation values of the full Hamiltonian, H, with respect to states, which, if H_2 is a good approximation to H, should be good first approximations to the eigenstates of H.

If H₂ is fairly complicated, the variationally optimal choices for the matrix elements of the transformation may be too complex to allow computation of expectation values of H. In this case the qualitative character of these optimal choices might be imitated by constructing relatively simple analytical forms containing variational parameters to be determined by the variational principle.

The previous discussion briefly outlines a variational method for obtaining approximate eigenvalues of a Hamiltonian which may be qualitatively simulated by a quadratic one of the type treated here and thereby accomplishes the final objective of this work.

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APPEXDIX 1

MATHEMATICAL DEVELOPMENTS

(A1,1) Canonical Linear Coordinate Transformations.

Let $q_1, q_2, \dots, q_j, \dots, q_N$ be a set of generalized coordinates for some physical system. Let the set of linear equations

$$q'_{j} = \sum_{j'=1}^{N} c_{jj} q_{j}$$

(A1,1;1)

define N linearly independent coordinates q_1, q_2, \dots, q_N . Let P₁, P₂, ..., P_N be momenta conjugate to q_1, q_2, \dots, q_N respectively and let

$$P_{j}' = \sum_{j'=1}^{N} d_{jj} \cdot P_{j}$$

(A1,1;2)

Then

$$[P_{j}, P_{j}] = [q_{j}, q_{j}] = 0$$

(A1,1;3)

and

$$\begin{bmatrix} p', q'_{j'} \end{bmatrix} = \sum_{n=1}^{N} \sum_{n'=1}^{N} d_{jn} C_{j'n'} \begin{bmatrix} p_n, q_{n'} \end{bmatrix}$$
$$= \sum_{n=1}^{N} \sum_{n'=1}^{N} d_{jn} C_{j'n'} \delta_{nn'} \left(\frac{\hbar}{i}\right)$$
$$= \frac{\hbar}{i} \sum_{n=1}^{N} d_{jn} C_{j'n}.$$

Therefore, p_1 , p_2 ,..., p_N will be canonically conjugate to q_1 , q_2 ,..., q_N respectively if and only if

$$\sum_{n=1}^{N} d_{jn} c_{j'n} = \delta_{jj'};$$

(A1,1;4)

i.e., the matrices c and d are inverse transposes of one another. That c and d are inverse transposes of each other implies and is implied by the fact that the inverses of c and d are inverse transposes of each other. Hence, if the transformation described by (Al,l;l)and (Al,l;2) is canonical, then (and only then) will its inverse be canonical. Also, if this transformation is canonical, and if c (or d) is orthogonal, then c = d since the inverse of an orthogonal matrix is its transpose; and conversely, if c = d so that the coordinates and momenta transform alike, then c must be orthogonal if the transformation is to be canonical.

(A1,2;1)

(A1,2) Reduction of the Order of a Determinant

It is required to show that

 $\|D_{yy'}\|_{N} = \|D_{ij}\|_{J}$

where

$$D_{\nu\nu'} = \delta_{\nu\nu'} - \sum_{k} Q_{k}(\nu) Q_{k}(\nu') ;$$

$$D_{ij} = \delta_{ij} - \sum_{\nu} Q_{i}(\nu) Q_{j}(\nu') ;$$

(A1,2;2)

lower case Greek symbols take on the values 1, 2, ..., N; lower case Latin symbols take on the values $1, 2, ..., J \leq N$; and $Q_k(v)$ are arbitrary functions of the indicated indices. Here, $|| \qquad ||_M$ represents the M x M determinant of the enclosed M x M matrix. One may regard an N x N matrix as representing a linear transformation of an N-dimensional vector space, V, and a J x J matrix, a linear transformation of a J-dimensional subspace V' of V.

Let $A_{\mu}(v)$ be the vth component of the μ th element of any complete orthonormal set of vectors in V chosen so that

(A1,2)

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$$Q_k(y) = \sum_m a_{m,k} A_m(y)$$

.(A1,2;3)

and

$$a_{k,m} = a_{m,k}$$

(A1,2;4)

Using (A1,2;3) and (A1,2;4), one may write

$$\sum_{\nu} Q_{i}(\nu) Q_{j}(\nu) = \sum_{k} a_{i,k} a_{j,k}.$$

(A1,2;5)

Since the determinate of a matrix is invariant under an orthogonal transformation, it follows that

$$\| D_{vv} \|_{v} = \| \sum_{vv} A_{\mu}(v) D_{vv} A_{\mu}(v) \|_{v}.$$

Use of (A1,2;2) and (A1,2;3) yields

$$\|D_{\nu\nu}\|_{N} = \|\sum_{\nu\nu'} A_{\mu}(\nu) \delta_{\nu\nu'} A_{\mu'}(\nu') - \sum_{k mm'} a_{m,k} a_{m',k} \sum_{\nu\nu'} A_{m}(\nu) A_{m'}(\nu) A_{\mu'}(\nu) A_{\mu'}(\nu) \|_{N}.$$

$$\|D_{yy'}\|_{N} = \|S_{\mu\mu'} - \sum_{kmm'} a_{m,k} a_{m',k} S_{m\mu} S_{m'\mu'}\|_{N}$$
$$= \|S_{ij} - \sum_{k} a_{i,k} a_{j,k}\|_{J}.$$

Substitution of (A1,2;5) into the above expression yields the desired results; namely,

$$\|D_{\nu\nu'}\|_{N} = \|D_{ij}\|_{J}$$
.

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APPENDIX 2

MISCELLANEOUS CALCULATIONS

(A2,1) Evaluation of 1(z) in (3,3;17)

The following is an evaluation of I(z), where

$$I(z) = PP \int_{-\infty}^{\infty} \phi_{z}(k) dk ,$$

(A2,1;1)

where

$$= \int_{\Xi}^{2} (k) = \frac{1}{(k^{2} + \mu^{2})(k^{2} + \mu^{2} - \Xi)}$$

(A2,1;2)

In order to use the method of residues to evaluate (A2,1;1), it is necessary to specify a branch of the square root function in (A1,1;2). Write

$$(k^{2}+\mu^{2})^{\frac{1}{2}} = (k+i\mu)^{\frac{1}{2}}(k-i\mu)^{\frac{1}{2}},$$

and define the branch of that function as follows:

(A2,1)

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(A2,1;3)

with respect to the following diagram.


Note that $\oint_{z}(k)$ has poles at $k = \pm i\mu$ and $k = \pm i \hbar \mu^{2} - z^{2}$ for $0 \le z < \mu$ and at $k = \pm i\mu$ and $k = \pm (z^{2} - \mu^{2})$ for $z \ge \mu$.

Consider the following path, P, of integration in the complex k-plane for $0 \le z \le \mu$.



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(A2,1)

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$$P = \{k = (x, y) | y = 0, -R \le x \le R\} U C_R U C_D U C_\mu,$$

where

$$C_{R} = \left\{ k = (x, y) \middle| x^{2} + y^{2} = R^{2}, 0 \le y \le R, \epsilon \le x \le R \text{ or } -R \le x \le -\epsilon \right\},$$
$$C_{D} = \left\{ k = (x, y) \middle| x = \pm \epsilon, \mu + \epsilon \le y \le R \right\}$$

and

$$C_{\mu} = \left\{ (k - i\mu) = r e^{i\theta} \middle| r = \varepsilon, -\frac{3\pi}{2} \lesssim \theta \lesssim \frac{\pi}{2} \right\}.$$
(A2, 1;4)

Then,

$$\begin{split}
 \end{bmatrix} (\Xi) &= \lim_{\substack{\epsilon \to 0 \\ R \to \infty}} \left\{ \oint_{P} \varphi_{\Xi}(k) dk - \int_{C_{R}} \varphi_{\Xi}(k) dk - \int_{C_{D}} \varphi_{\Xi}(k) dk - \int_{T_{\Xi}} \varphi_{\Xi}(k) dk \right\} \\
 (A2, 1; 5)
 \end{split}$$

for $0 \le z \mu$.

Note that

$$\lim_{R\to\infty}\int_{C_R} \varphi_2(k)dk = 0.$$

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Now,

$$\lim_{\epsilon \to 0} \int_{\mathcal{F}_{z}} f(\mathbf{k}) d\mathbf{k} = \lim_{\epsilon \to 0} \int_{\mathcal{C}_{\mu}} \frac{d\mathbf{k}}{(\mathbf{k}^{2} + \mu^{2})(1\mathbf{k}^{2} + \mu^{2} - \mathbf{z})}$$

$$= \int_{\pi/2}^{-3\pi/2} \frac{i\epsilon e^{i\Theta} d\Theta}{(2i\mu)\epsilon e^{i\Theta}(-\mathbf{z})}, \ \mathbf{z} \neq 0,$$

or

$$\lim_{\epsilon \to 0} \int_{C_{\mu}} \Phi_{z}(k) dk = \frac{\pi}{\mu z}, z \neq 0.$$
(A2,1;6)

Consider the integration over the contour, C_{D} .

$$\begin{split} \lim_{E \to O} \int_{C_{D}} \varphi_{z}(k) dk &= \lim_{E \to O} \int_{C_{D}} \frac{dk}{(k^{2} + \mu^{2})(k^{2} + \mu^{2} - z)} \\ &= \int_{R}^{\mu} \frac{i \, dy}{(\mu^{2} - \gamma^{2})(i \sqrt{\gamma^{2} - \mu^{2}} - z)} + \int_{\mu}^{R} \frac{i \, dy}{(\mu^{2} - \gamma^{2})(i \sqrt{\gamma^{2} - \mu^{2}} - z)} \\ &= i \int_{\mu}^{R} \frac{dy}{(\mu^{2} - \gamma^{2})} \left[\frac{1}{\overline{z} - i \sqrt{\gamma^{2} - \mu^{2}}} - \frac{1}{\overline{z} + i \sqrt{\gamma^{2} - \mu^{2}}} \right] \\ &= 2 \int_{\mu}^{R} \frac{dy}{\sqrt{\gamma^{2} - \mu^{2}}} \left[\frac{y^{2} - (\mu^{2} - \overline{z}^{2})}{\sqrt{\gamma^{2} - \mu^{2}}} \right] \cdot \end{split}$$

$$(A2, 1; 7)$$

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(A2,1)

Let $y = \mu \sec \theta (dy = \mu \tan \theta \sec \theta d\theta)$. Then,

$$\lim_{\substack{\epsilon \to 0 \\ R \to \infty}} \int_{C_{D}} \mathcal{A}_{k}(k) dk = 2 \int_{0}^{\frac{\mu}{2}} \frac{\mu \tan \theta \sec \theta d\theta}{\mu \left[\sec^{2} \theta - 1 \left[\mu^{2} \sec^{2} \theta - (\mu^{2} - Z^{2}) \right] \right]}$$

$$= 2 \int_{0}^{\frac{\pi}{2}} \frac{\cos \theta \, d\theta}{\cos^2 \theta \left[\frac{\mu^2}{\cos^2 \theta} - \left(\frac{\mu^2 - z^2}{z^2} \right) \right]}$$

$$=2\int_{0}^{1/2}\frac{\cos\theta\,d\theta}{\left[\mu^{2}-(\mu^{2}-z^{2})\cos^{2}\theta\right]}$$

Let $x = \sin \theta (dx = \cos \theta d\theta)$. Then,

$$\lim_{\substack{E \to 0 \\ R \to \infty}} \oint_{C_{p}} \varphi_{z}(k) dk = 2 \int_{0}^{1} \frac{dx}{\left[\mu^{2} - (\mu^{2} - \overline{z}^{2})(1 - x^{2})\right]}$$
$$= 2 \int_{0}^{1} \frac{dx}{\left[\overline{z}^{2} + (\mu^{2} - \overline{z}^{2})x^{2}\right]}$$
$$= \frac{2}{(\mu^{2} - \overline{z}^{2})} \int_{0}^{1} \frac{dx}{\left[x^{2} + \overline{z}^{2}/(\mu^{2} - \overline{z}^{2})\right]}$$
$$= \frac{2}{\overline{z} - \overline{\mu^{2} - \overline{z}^{2}}} \tan^{-1} \left(\frac{-1}{\overline{\mu}^{2} - \overline{z}^{2}}\right)$$

for $0 < z < \mu$.

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(A2,1;8)

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(A2,1)

The integration over the contour P has a contribution coming from the single simple pole at $k = +i \left(\frac{\mu^2 - z^2}{\mu^2 - z^2} \right)$. Thus,

\$

$$\lim_{\substack{\epsilon \to 0 \\ R \to \infty}} \oint_{P} \mathcal{A}_{\sharp}(k) dk = 2\pi i R_{\circ},$$

where

. .

$$R_{o} = \left[\frac{Z + \sqrt{k^{2} + \mu^{2}}}{(k^{2} + \mu^{2})(k + i\sqrt{\mu^{2} - Z^{2}})}\right]_{k = i\sqrt{\mu^{2} - Z^{2}}}$$
$$= \frac{1}{iZ + \sqrt{\mu^{2} - Z^{2}}}, \quad Z \neq 0.$$

$$\lim_{E \to 0} \oint_{P} \varphi_{z}(k) dk = \frac{2\pi}{Z \sqrt{\mu^{2} - Z^{2}}}, \quad 0 < z < \mu.$$
(A2, 1;9)

If one substitutes (A2,1;9), (A2,1;8), and (A2,1;6) into (A2,1;5), one obtains

$$I(z) = \frac{2\mu \left[\pi - \tan^{-1} \left(\frac{1\mu^2 - z^2}{z} \right) \right] - \pi - \mu^2 - z^{2^2}}{\mu z \left[\mu^2 - z^2 \right]}, \quad 0 \le z < \mu.$$

(A2,1;10)

(A2,1)

Note that in (A2,1;10) I(O) is indeterminant of the form $\frac{0}{0}$. However, L'Hospital's rule may be employed to obtain

$$I(0) = \frac{2}{\mu^2}$$
 (A2, 1; 11)

To evaluate I(z) in (A2,1;1) for $z \ge \mu$, let

$$Z = - \left[\frac{k_o^2 + \mu^2}{k_o + \mu^2} \right], \quad k_o \ge 0.$$

(A2, 1; 12)

Consider the following contour P' in the complex k-plane.

$$P' = \begin{cases} -R \leq x \leq -k_o - \epsilon', \\ k = (x, y) \end{cases} y=0, \text{ or } -k_o + \epsilon' \leq x \leq k_o - \epsilon' \\ \text{ or } k_o + \epsilon' \leq x \leq R \end{cases} UC_R UC_D UC_\mu UCUC^{\dagger},$$

where

•

$$C^{-} = \left\{ k \mid k = -k_{\circ} + \epsilon' e^{i\theta}, \epsilon' > 0, 0 \le \theta \le \pi \right\},$$
$$C^{+} = \left\{ k \mid k = k_{\circ} + \epsilon' e^{i\theta}, \epsilon' > 0, 0 \le \theta \le \pi \right\},$$

and $C_R^{},\ C_D^{},\ and\ C_{}_{\mu}$ are as defined in (A2,1;4). The path P' is diagramed as:

(A2,1)



Exactly as before,



so that

$$I(\overline{z}) = \lim_{\substack{\epsilon \to 0 \\ \epsilon' \to 0 \\ R \to \infty}} \left\{ \oint_{P'} \mathcal{A}_{\underline{z}}(k) dk - \int_{C_{D}} \mathcal{A}_{\underline{z}}(k) dk - \int_{C_{\mu}} \mathcal{A}_{\underline{z}}(k) dk - \int_{C_{\mu}} \mathcal{A}_{\underline{z}}(k) dk - \int_{C_{\mu}} \mathcal{A}_{\underline{z}}(k) dk \right\}, \quad \overline{z} \ge \mu.$$

$$(A2, 1; 13)$$

In the same manner as done previously it may be shown that

$$\lim_{\epsilon \to 0} \int \varphi_{\pm}(k) dk = \frac{\pi}{\mu \Xi} \cdot (A2, 1; 14)$$

(A2,1)

To evaluate the integrals over the contours $\ensuremath{\mathsf{C}}^{-}$ and $\ensuremath{\mathsf{C}}^{+}$ note that

$$\oint_{\mathbb{Z}}(k) \xrightarrow{k \to \pm k_{o}} \pm \frac{1}{k_{o} - k_{o}^{2} + \mu^{2}}(k \pm k_{o})$$

(A2,1;15)

From (A2,1;15) it follows that

$$\lim_{\varepsilon' \to 0} \int_{C^{-}} \varphi_{\underline{z}}(k) dk = \frac{-1}{k_0 \left[k_0^2 + \mu^2\right]} \int_{C^{-}} \frac{dk}{k - k_0}$$
$$= \frac{-1}{k_0 \left[k_0^2 + \mu^2\right]} \int_{T} \frac{i\varepsilon' e^{i\Theta} d\Theta}{\varepsilon' e^{i\Theta}}$$

$$=\frac{i\pi}{k_{o}\tau k_{o}^{2}+\mu^{2}},$$

and

.

$$\lim_{\substack{\epsilon' \to 0 \\ c^+}} \int_{c^+} \frac{1}{k_0 \sqrt{k_0^2 + \mu^{2^1}}} \int_{c^+} \frac{dk}{k + k_0}$$
$$= \frac{1}{k_0 \sqrt{k_0^2 + \mu^{2^1}}} \int_{T} \frac{i\epsilon' e^{i\Theta} d\Theta}{\epsilon' e^{i\Theta}}$$
$$= \frac{-i\pi}{k_0 \sqrt{k_0^2 + \mu^{2^1}}}.$$

Therefore,

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$$\lim_{\epsilon' \to 0} \left\{ \int_{C^*} \varphi_{\underline{z}}(k) dk + \int_{C^+} \varphi_{\underline{z}}(k) dk \right\} = 0.$$

(A2,1;16)

Now

$$\lim_{E \to 0} \int_{C_{D}} \mathcal{A}_{\Xi}(k) dk = \lim_{E \to 0} \int_{C_{D}} \frac{dk}{(k^{2} + \mu^{2})(1k^{2} + \mu^{2} - \Xi)}$$
$$= \int_{R}^{\mu} \frac{i \, dy}{(\mu^{2} - \gamma^{2})(1\sqrt{2} - \mu^{2} - \Xi)} + \int_{\mu}^{R} \frac{i \, dy}{(\mu^{2} - \gamma^{2})(-i \sqrt{2} - \Xi)}$$
$$= 2 \int_{\mu}^{R} \frac{dy}{(1\sqrt{2} - \mu^{2})[\gamma^{2} + (\Xi^{2} - \mu^{2})]}.$$

Let $y = \mu$ sec θ . Then,

$$\lim_{E \to 0} \int_{C_0} \Psi_{\underline{z}}(k) dk = 2 \int_{0}^{\frac{\pi}{2}} \frac{\mu \tan \Theta \sec \Theta d\Theta}{\mu \left[\sec^2 \Theta - 1 \left[\mu^2 \sec^2 \Theta + \left(\underline{z}^2 - \mu^2 \right) \right]},$$

or

•

$$\lim_{\epsilon \to 0} \int_{C_{D}} \mathcal{A}_{z}(k) dk = 2 \int_{C_{D}} \frac{\cos \theta d\theta}{\left[\mu^{2} + (z^{2} - \mu^{2})\cos^{2}\theta\right]}.$$

Let $x = \sin \theta$, so that

$$\lim_{E \to 0} \int_{C_D} \mathcal{I}_{z}(k) dk = \frac{2}{(z^2 - \mu^2)} \int_{0}^{1} \frac{dx}{[z^2 - \mu^2] - x^2]} dx$$

$$\lim_{\substack{E \to 0 \\ R \to \infty}} \int_{C_0} \varphi_{\underline{z}}(k) dk = \frac{1}{\overline{z} - \overline{z^2 - \mu^2}} \log \left(\frac{\overline{z} + \overline{z^2 - \mu^2}}{\overline{z} - \overline{z^2 - \mu^2}} \right).$$

(A2,1;17)

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Since the path P' encloses no poles of the integrand of l(z), it follows that

$$\oint_{\mathbf{P}} \Phi_{\mathbf{z}}(\mathbf{k}) d\mathbf{k} = 0$$
(A2, 1; 18)

Substitution of (A2,1;18), (A2,1;17), (A2,1;16), and (A2,1;14) into (A2,1;13) yields

$$\left[(Z) = -\left[\frac{TT}{\mu Z} + \frac{1}{Z + Z^2 - \mu^2} log \left(\frac{Z + (Z^2 - \mu^2)}{Z - (Z^2 - \mu^2)} \right) \right], Z \ge \mu.$$
(A2, 1; 19)

One may use L'Hospital's rule on the indeterminant form in (A2,1;19) to obtain

$$J(\mu) = -\frac{(\pi - 2)}{\mu^2} - \frac{(\pi - 2)}{\mu^2} - \frac{$$

Combining (A2,1;20), (A2,1;19), (A2,1;11), and (A2,1;10) gives the result quoted in (3,3;19).

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(A2,2) Evaluation of g_2 in (3,4;39)

The method of (3,2) is to be applied to the evaluation of g_2 as given in (3,4;39), i.e.

$$q_{2} = \frac{1}{2} \left[\sum_{\gamma} \Omega_{\gamma} - \sum_{\vec{k}} \omega(\vec{k}) \right], \qquad (A2, 2; 1)$$

where

and the Ω_{v}^{2} 's are solutions for Ω^{2} of the secular equation,

$$\left| \left(\Omega^2 - \omega^2(k) \right) \delta_{\vec{k}\cdot\vec{k}} - 4 - \left[\omega(k) \omega(\vec{k}) \left(\vec{k}\cdot\vec{k} \right) f_k f_{\vec{k}} \right] \right| = 0, \qquad (A2, 2; 3)$$

or

$$\left\| \left(\Omega^2 - \omega^2(k) \right) \delta_{\vec{k}\vec{k}} - \vec{F}(\vec{k}) \cdot \vec{F}(\vec{k}) \right\| = 0,$$

(A2,2;4)

where

$$\vec{F}(\vec{k}) = 2 \vec{k} t \omega(\vec{k}) f_k$$
.

(A2,2;5)

Following the procedure outlined in (3,2), one may write

$$g_2 = \frac{1}{4\pi i} \oint_P d z f \overline{z} \left[\sum_{\nu} \frac{1}{\overline{z} - \Omega_{\nu}^2} - \sum_{\overline{k}} \frac{1}{\overline{z} - \omega^2(k)} \right],$$

where

$$\overline{Z} = + \overline{\Pi Z \Pi} e^{\frac{i}{2} \operatorname{ang} Z} , - \pi < \operatorname{ang} Z \leq \pi ,$$

and P is the contour shown in the following diagram.



(A2,2)

For all z not on L define

$$J(z) = \prod_{k} (z - \Omega_{v}^{2}) = ||(z - \Omega_{v}^{2}) \delta_{vv'}||$$
$$= ||(z - \omega^{2}(k)) \delta_{\vec{k}\vec{k}'} - \vec{F}(\vec{k}) \cdot \vec{F}(\vec{k}')||,$$
$$J_{o}(z) = \prod_{k} (z - \omega^{2}(k)) = ||(z - \omega^{2}(k)) \delta_{\vec{k}\vec{k}'}||,$$

and

$$\Gamma(\overline{z}) = \frac{J(\overline{z})}{J_{o}(\overline{z})} = \frac{1}{\prod_{k} (\overline{z} - \omega^{2}(k))} \left\| (\overline{z} - \omega^{2}(k)) \delta_{\overline{k}\overline{k}'} - \overline{F}(\overline{k}) \cdot \overline{F}(\overline{k}') \right\|$$

$$= \left\| \delta_{\overline{k}\overline{k}'} - \frac{\overline{F}(\overline{k}) \cdot \overline{F}(\overline{k})}{|\overline{z} - \omega^{2}(k)|} \right\|. \quad (A2, 2; 6)$$

Then,

$$g_2 = \frac{1}{4\pi i} \oint_P dz f \overline{z} \frac{d}{dz} \log \Gamma(\overline{z}),$$

or

$$g_2 = -\frac{1}{8\pi i} \oint dz \frac{1}{1Z} \log \Gamma(z). \qquad (A2,2;7)$$

In expression (A2,2;6) for $\Gamma(z)$ let

$$Q_{i}(\vec{k}) = \frac{F_{i}(\vec{k})}{1 z - \omega^{2}(k)} .$$

(A2,2;8)

Then,

$$\int \overline{(z)} = \left\| \delta_{\vec{k}\vec{k}} - \sum_{i=1}^{3} Q_{i}(\vec{k}) Q_{i}(\vec{k}') \right\|,$$

or .

$$[T_{(z)} = \| \delta_{ij} - \sum_{\vec{k}} Q_i(\vec{k}) Q_j(\vec{k}) \|.$$

(A2,2;9)

Because of the symmetry of $Q_i(\vec{k})$,

$$\sum_{\vec{k}} Q_i(\vec{k}) Q_j(\vec{k}) = \begin{cases} 0, & \text{if } i \neq j \\ \sum_{\vec{k}} Q_3(\vec{k}) Q_3(\vec{k}), & \text{if } i = j \end{cases}$$

Thus,

$$\Gamma(z)=r^{3}(z),$$

where

$$r(z) = 1 - \sum_{\vec{k}} Q_3(\vec{k}) Q_3(\vec{k}).$$

Hence,

$$g_2 = -\frac{3}{8\pi i} \oint_P dz \frac{1}{12} \log r(z).$$

(A2,2;10)

(A2,2)

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Making the replacement

$$\sum_{\vec{k}} \xrightarrow{S \to \infty} \frac{S}{8\pi^3} \int d^3 \vec{k} ,$$

$$\Gamma(Z) \xrightarrow{S \to \infty} |-\frac{S}{3\pi^2} \int_{-\infty}^{\infty} \frac{k^4(1+k^2)f_k^2 dk}{Z - (1+k^2)^2},$$

where \boldsymbol{f}_k is given by (3,4;21) and (3,4;2) as

$$f_{k} = \sqrt{\frac{4\pi\alpha}{S}} \frac{\lambda k_{o}^{2}}{k(k^{2} + k_{o}^{2})}$$

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Let z = x + iy. Since the integrand in (A2,2;10) is analytic above and below the real axis, and on the real axis between 0 and 1, let the path P approach the locus L. Then,

$$Q_2 = \frac{3}{8\pi i} \int dx \frac{1}{1x} \log \frac{r_+(x)}{r_-(x)}$$
, (A2,2;11)

where

$$f_{\pm}(x) = \lim_{y \to 0} \Gamma(x \pm iy)$$

$$\frac{S \to \infty}{Y \to 0} | + \lim_{y \to 0} \frac{S}{3\pi^2} \left(\frac{4\pi\alpha}{S} \right) \chi^2 k_0^4 \int_{-\infty}^{\infty} \frac{k^2 (1+k^2) dk}{\left[\left((1+k^2)^2 - (x \pm iy) \right] \left(k^2 + k_0^2 \right)^2 \right]} dk$$

or

$$f_{\pm}(x) = 1 + \frac{4\alpha \lambda^2 k_{\bullet}^4}{3\pi} \int_{-\infty}^{\infty} \Phi_{\pm}(k) dk$$

where

$$\Phi_{\pm}(k) = \frac{k^{2}(1+k^{2})}{(k^{2}+k^{2}_{o})^{2}(k^{2}+b^{2})(k^{2}-a^{2}_{\pm})}$$

and

$$b = f(x' + 1)$$

$$a_{\pm} = f(x \pm iy' - 1) \xrightarrow{y \to 0} a = f(x' - 1).$$
(A2, 2; 12)

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Hence, using the method of residues to calculate $r_{\pm}(x)$ yields

$$Y_{\pm}(x) = 1 + 2\pi i \left[R_1 + R_2 \pm R_3 \right],$$

where

$$R_{1} = \frac{1}{2!} \left\{ \frac{d}{dk} \left[\frac{k^{2}(1+k^{2})}{(k+ik_{o})^{2}(k^{2}+b^{2})(k^{2}-a^{2})} \right] \right\}_{k=ik_{o}}$$

$$= \frac{1}{2} \left\{ \frac{4k_{o}^{2}(1-k_{o}^{2}) + (3k_{o}^{2}-1)(b^{2}-k_{o}^{2})(a^{2}+k_{o}^{2})}{4ik_{o}(b^{2}-k_{o}^{2})^{2}(a^{2}+k_{o}^{2})^{2}} \right\},$$

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$$R_{2} = \left[\frac{k^{2}(1+k^{2})}{(k^{2}+k^{2})^{2}(k+ib)(k^{2}-a^{2})}\right]_{k=ib}$$
$$= \left[\frac{b(1-b^{2})}{2i(b^{2}-k^{2})^{2}(a^{2}+b^{2})}\right],$$

and

$$R_{3} = \lim_{y \neq 0} \left[\frac{k^{2}(1+k^{2})}{(k^{2}+k^{2})^{2}(k^{2}+b^{2})(k+a_{\pm})} \right]_{k=a_{\pm}} = \left[\frac{a(1+a^{2})}{2(a^{2}+k^{2})^{2}(a^{2}+b^{2})} \right].$$

Using (A2,2;12) and the replacement,

$$w = 1x - 1$$
,

yields

$$Y_{\pm}(w) = X(w) \pm i Y(w)$$

where

$$X(w) = \left| + \frac{2\alpha k_o^3 \lambda^2}{3} \left[\frac{4k_o^2 (1-k_o^2)^2 + (3k_o^2 - 1)(w^2 + 2 - k_o^2)(w^2 + k_o^2) - k_o (w^2 + 2 - k_o^2)}{(w^2 + 2 - k_o^2)^2 (w^2 + k_o^2)^2} \right]$$

and

$$Y(w) = \frac{2\alpha k_{o}^{4} \lambda^{2}}{3} \left[\frac{w}{(w^{2} + k_{o}^{2})^{2}} \right].$$

(A2,2;13)

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(A2,2)

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(A2,2)

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Hence,

$$g_z = \frac{3}{\pi} \int_{0}^{\infty} dw \ w \ (w)$$

where

$$H(w) = \operatorname{arg} \left[X(w) + i Y(w) \right],$$

(A2,2;14)

and X(w) and Y(w) are given in (A2,2;13). This is the result for g_2 given in (3,4;41) through (3,4;44).

(A2,3) Expansion of g_2 in (3,4;41) for Weak Coupling

Referring to (A2,2;13) and (A2,2;14) for g , one may write to first order in α ,

$$\frac{\Upsilon(w)}{\chi(w)} \xrightarrow{\alpha \to 0} \frac{2\alpha k_o^4 \lambda^2}{3} \left[\frac{w}{(w^2 + k_o^2)^2} \right].$$
(A2,3;1)

Hence

$$(H)(w) \xrightarrow{\alpha \to 0} \tan^{-1}\left(\frac{Y(w)}{X(w)}\right) \xrightarrow{\alpha \to 0} \frac{2\alpha k_o^4}{3} \left[\frac{w}{(w^2 + k_o^2)^2}\right].$$

$$g_2 = \frac{2\alpha k_0^4 l^2}{\pi} \int_{0}^{\infty} \frac{w^2 dw}{(w^2 + k_0^2)^2} dw$$

(A2,3)

(A2,3;2)

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 $Q_2 = \frac{\alpha k_o^+ \lambda^2}{TT} \int_{-\infty}^{\infty} \frac{w^2 dw}{(w^2 + k_o^2)^2} \cdot$

Evaluation of (A2,3;2) by the method of residues yields

$$g_2 = \frac{\alpha k_o^2 2^2}{\Pi} (2 \pi i) \left(\frac{1}{2!}\right) \left[\frac{d}{dw} \left(\frac{w^2}{(w+ik_o)^2}\right)\right]_{w=ik_o},$$

or

$$q_2 = \frac{\alpha k_o^3 \lambda^2}{2};$$

(A2,3;3)

Using (A2,2;13) one may write to second order in α ,

$$\frac{Y(w)}{X(w)} \xrightarrow{\alpha \to 0} \frac{b\alpha}{1 + a\alpha}$$

$$= b\alpha - ab\alpha^{2} + O(\alpha^{3}), \qquad (A_{2}, 3; 4)$$

where

and

$$b = \frac{2 k_{o}^{4} \lambda^{2} w}{3 (w^{2} + k_{o}^{2})^{2}}$$

$$Q = \frac{2k_{o}^{3}\chi^{2}}{3} \left[\frac{4k_{o}^{2}(1-k_{o}^{2})^{2} + (3k_{o}^{2}-1)(w^{2}+2-k_{o}^{2})(w^{2}+k_{o}^{2}) - k_{o}\sqrt{w^{2}+2}(w^{2}+k_{o}^{2})^{2}}{(w^{2}+2-k_{o}^{2})^{2}(w^{2}+k_{o}^{2})^{2}} \right] \right]$$
(A2.3:5)

or

(A2,3)

Using (A2,3;4) and (A2,2;14), one may express g_2 as

$$g_2 = \frac{3}{\pi} \int_{0}^{\infty} dw \ w \ \tan^{-1}\left(\frac{Y(w)}{X(w)}\right)$$

$$=\frac{3}{\pi}\int_{0}^{\infty}dw w \left[b\alpha - ab\alpha^{2} + O(\alpha^{3})\right],$$

or

$$g_{2} = \left[\frac{3}{\pi}\int_{\alpha}^{\infty} dw w b\right] \alpha - \left[\frac{3}{\pi}\int_{\alpha}^{\infty} dw w a b\right] \alpha^{2} + O(\alpha^{3}),$$
(A2,3;6)

where a and b are given by (A2,3;5).

The first term in (A2,3;6) is the one just previously evaluated and is thus given by (A2,3;3). Therefore,

$$f_2 = \frac{k_0^3 l^2}{2} \alpha - g_2 \alpha^2 + O(\alpha^3),$$

(A2,3;7)

where

$$g_2' = \frac{3}{\pi} \int_{\alpha}^{\infty} ab w dw,$$

(A2,3;8)

a and b given by (A2,3;5).

In (A2,3;7), g_2' is needed only to zeroth order in α . Hence, it is sufficient to calculate g_2' using the zeroth order

(A2,3)

optimum values of $k_{\mbox{\scriptsize o}}$ and $\lambda,$ i.e.,

Then

$$q_2' = l_o - l_1,$$

where

$$\mathcal{L}_{o} = \frac{4}{3\pi} \int_{-\infty}^{\infty} \frac{w^{2} dw}{(w^{2}+1)^{2}}$$
(A2,3;10)

and

$$l_{1} = \frac{4}{3\pi} \int_{0}^{\infty} \frac{w^{2} - w^{2} + 2}{(w^{2} + 1)^{4}} dw - (A2, 3; 11)$$

Evaluation of (A2,3;10) by the method of residues yields

 $l_o = \frac{1}{12}$ (A2,3;12)

In (A2,3;11) let $w = \sqrt{2}$ tan θ . Then,

$$l_{1} = \frac{4}{3\pi} \int_{0}^{\frac{\pi}{2}} \frac{4\tan^{2}\Theta \tan^{2}\Theta + 1}{\left[2\tan^{2}\Theta + 1\right]^{4}}$$

$$=\frac{16}{3\pi}\int_{0}^{\frac{\pi}{2}}\frac{\sin^{2}\Theta\cos^{3}\Theta}{\cos^{2}\Theta\left[2\frac{\sin^{2}\Theta}{\cos^{2}\Theta}+1\right]^{4}}$$

(A2,3;9)

$$L_1 = \frac{16}{3\pi} \int_{0}^{\frac{\pi}{2}} \frac{\sin^2\theta \left(1 - \sin^2\theta\right) \cos\theta d\theta}{\left[1 + \sin^2\theta\right]^4}$$

Let $x = \sin \theta$. Then,

$$\mathcal{L}_{1} = \frac{16}{3\pi} \int_{0}^{1} \frac{x^{2}(1-x^{2}) dx}{(x^{2}+1)^{4}}$$
$$= \frac{16}{3\pi} \left\{ \frac{x^{3}}{3(1+x^{2})^{3}} \right|_{0}^{1}$$

.

or'

$$l_{1} = \frac{16}{3\pi} \left(\frac{1}{3 \cdot 2^{3}} \right) = \frac{2}{9\pi} \, .$$

(A2,3;13)

Substituting (A2,3;13) and (A2,3;12) into (A2,3;10), one obtains

$$q_2' = \left(\frac{1}{12} - \frac{2}{9\pi}\right),$$

or

$$g'_2 = 0.0126$$
.

(A2, 3; 14)

Hence, combining (A2,3;14) and (A2,3;7) yields

$$g_2 = \frac{k_a^3 \chi^2}{2} \alpha - 0.0126 \alpha^2 + O(\alpha^3).$$

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(A2,3)

Substitution of this result into equation (3,4;37) for E_0 and minimization of the result with respect to k_0 and λ still yield $k_0 = \lambda = 1$. Hence, to second order in α , g_2 is given by

$$g_2 = \frac{\alpha}{2} = 0.0126 \alpha^2 + O(\alpha^3).$$

(A2,3;7)

(A2,3)

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EXAMINATION AND THESIS REPORT

Candidate: James Lannis Roberts

Major Field: Physics

Title of Thesis: A Systematic Study and Applications of the Eigenvalue Problem for Quadratic Hamiltonians

Approved:

Major Professor and Chairman

Dean of the Graduate School

EXAMINING COMMITTEE:

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