Diagonalization Procedure for a Bose System Hamiltonian

Kowalska, A.; Lindgård, Per-Anker

Publication date: 1966

Document Version
Publisher's PDF, also known as Version of record

Link back to DTU Orbit

Citation (APA):
Diagonalization Procedure for a Bose-System Hamiltonian

by Antonina Kowalska and P.A. Lindgård Mogensen

May, 1966

Sales distributor: Jul. Gjellerup, 87, Sølvgade, Copenhagen K, Denmark
Available on exchange from: Library, Danish Atomic Energy Commission, Risø, Roskilde, Denmark
Diagonalization Procedure for a Bose-System Hamiltonian

by

Antonina Kowalska
University Jagiellońska
Institute of Physics
Kraków, Poland

and

P. A. Lindgård Mogensen
The Danish Atomic Energy Commission
Research Establishment Risø
Physics Department

Abstract

A diagonalization procedure for a quadratic form of Bose operators is presented. Explicit, exact expressions for the eigenvalues and the transformation matrices are given for the case of two interacting Bose systems. As examples of applications may be mentioned simple magnon treatment of antiferromagnets or ferromagnets with two atoms per unit cell, magnon-phonon interaction and other interactions between collective modes.
## Contents

<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Introduction</td>
<td>3</td>
</tr>
<tr>
<td>1. Diagonalization of a General Bilinear, Two-Bose-System Hamiltonian</td>
<td>3</td>
</tr>
<tr>
<td>2. Method of Finding the Coefficients of the Transformation Matrix $T$</td>
<td>9</td>
</tr>
<tr>
<td>3. Conclusion</td>
<td>20</td>
</tr>
<tr>
<td>Acknowledgement</td>
<td>20</td>
</tr>
<tr>
<td>Appendix 1. Calculation of Energies in the Third Case</td>
<td>21</td>
</tr>
<tr>
<td>Appendix 2. Explicit Calculation of the Matrix $T$ for a Special Case</td>
<td>23</td>
</tr>
<tr>
<td>References</td>
<td>30</td>
</tr>
</tbody>
</table>
Introduction

By diagonalization of a Hamilton operator we mean a procedure for finding the energy eigenvalues and the coefficients of the matrix which transforms the Hamiltonian into its diagonal form. In physical applications the energy values are usually of principal interest, and there exist relatively simple methods of obtaining them; well known is the Bogoliubov equation-of-motion method. We shall here present a method which is a slight generalization of the simple diagonalization method of a symmetric quadratic form.

In the literature, the coefficients of the transformation matrix are given explicitly only for some special cases. It appears that the coefficients play a role in obtaining information about the interaction in a Bose system. This is the case with the magnon treatment of the rare-earth metals discussed in ref. 2. Therefore we shall give a procedure and the explicit expressions for the coefficients for more general cases which appear to be of importance for instance in spin-wave analysis of materials having non-isotropic spin interaction. The procedure may be characterized as a step-transformation method.

In section 1 we give the eigenvalues of a general bilinear, two-Bose-system Hamiltonian, and in section 2 the step-transformation matrices are given for a number of cases.

In appendix 2 we illustrate the step-transformation method by calculating the final transformation matrix in a simple case.

1. Diagonalization of a General Bilinear, Two-Bose-System Hamiltonian

Let us for simplicity give the calculations for two interacting Bose systems, "a" and "b", with equal numbers of particles. One may think of systems like ferromagnets with two atoms per unit cell, antiferromagnets, magnon-phonon systems, etc. The theory might easily be extended to deal with more than two systems.

The most general Hamiltonian bilinear in Bose operators we are going to consider may be written

\[ H_{\text{tot}} = \sum_{q} H'_{q} ; \]  

(1.1)
q is short for wave vector \( \vec{q} \).

\[
H_q' = \frac{1}{2} A^a_q (a^+_q a_q + a_q^+ a^-_q )
+ \frac{1}{2} A^b_q (b^+_q b_q + b_q^+ b^-_q )
+ \frac{1}{2} (B^a_q a_q^+ - a^-_q a_q^+ )
+ \frac{1}{2} (B^b_q b_q^+ - b^-_q b_q^+ )
+ C^q q^+ b_q^+ q^+ b^+_q
+ D^q q^+ b^-_q q^+ b^-_q
\]

\( A^a,^b_q \) is real because \( H_q' \) must be hermitian;

\( B^a,^b_q = B^a,^b_q^\ast \) because of the Bose commutation relations (BCR) and the symmetrization performed.

The coefficients \( A^a_q \), \( B^a_q \), \( C_q \), and \( D_q \) are defined through (1.2) and are at the beginning subject to no more restrictions.

Let us write (1.1) in a more systematic way as

\[
H_{\text{tot}} = \Sigma_{q} H_q' = \Sigma_{q} H_q,
\]

where

\[
H_q = \frac{1}{2} \left[ \begin{array}{cccc}
A^a_q & B^{a^\ast}_q & C^q & D^{a^\ast}_q \\
B^a_q & A^q & D^q & C^q \\
C^q & D^q & A^q & B^{b^\ast}_q \\
D^q & C^q & B^{a^\ast}_q & A^q \\
\end{array} \right] \left[ \begin{array}{c}
a_q \\
an^+_q \\
b_q \\
b^{\ast}_q \\
\end{array} \right]
\]

or in short notation

\[
H_q = \frac{1}{2} A^+ \ H \ A ,
\]
where $H$ is the $4 \times 4$ matrix and $A$ the "column operator". $H_q = H_q^{+}$ because $H$ is hermitian.

We want to diagonalize (1.1) for an arbitrary $q$. So let us assume that for this $q$ there exists a non-singular transformation matrix $T$ (short for $T_q$) so that

$$H_q = \frac{1}{2} A^+ H_q A = \frac{1}{2} (T^{-1} A)^+ T^+ H T (T^{-1} A)$$

$$= \frac{1}{2} F^+ E F,$$

where $E$ is a diagonal matrix,

$$E = T^+ H T, \quad \text{and} \quad A = T F.$$

We define the second equality in (1.7) explicitly by

$$\begin{align*}
\begin{pmatrix}
a_q \\
 a_{-q}^+ \\
b_q \\
b_{-q}^+
\end{pmatrix}
&= \begin{pmatrix}
a_1 & a_2 & a_3 & a_4 \\
\beta_2 & \beta_1 & \beta_4 & \beta_3 \\
\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
\delta_2 & \delta_1 & \delta_4 & \delta_3
\end{pmatrix}
\begin{pmatrix}
F_q \\
F_{-q}^+ \\
G_q \\
G_{-q}^+
\end{pmatrix}
\end{align*}$$

(1.8)

where $F_q$ and $G_q$ are quasi-particle operators and the $q$-dependent coefficients are defined in such a way that $a_i(-q) = \beta_i(q)$ and $\gamma_i(-q) = \delta_i(q)$.

(1.8) expresses that we want to diagonalize $H_{tot}$ by writing every operator as a linear combination of some quasi-particle operators. The matrix $E$ is defined by

$$H_q = \frac{1}{2} F^+ E F = \frac{1}{2} \left( F_q^+ F_{-q} G_q^+ G_{-q} \right).$$

(1.9)
\[ E_{\omega, q}^f, g \] is real because \( q = \frac{1}{2} \).

The total Hamiltonian will then assume the diagonal form (1.11):

\[
H_{\text{tot}} = \frac{1}{2} \sum_{q \text{ all}} (E_q^f F_q^+ F_q + E_q^f F_q^+ F_q + E_q^g G_q^+ G_q + E_q^g G_q^+ G_q) \quad (1.10)
\]

\[
= \sum_{q \text{ all}} [\hbar \omega_q^f (F_q^+ F_q + \frac{1}{2}) + \hbar \omega_q^g (G_q^+ G_q + \frac{1}{2})], \quad (1.11)
\]

where \( \hbar \omega_q^f, g = E_q^f, g \) are the dispersion relations for the two possible modes described by \( F_q \) and \( G_q \) operators. To obtain this result we have used the fact that all operators involved are Bose operators.

By combining (BCR) and (1.9) one sees that the coefficients in the \( T \) matrix must fulfill the equation

\[
\begin{pmatrix}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\
\beta_1 & \beta_2 & \beta_3 & \beta_4 \\
\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
\delta_1 & \delta_2 & \delta_3 & \delta_4
\end{pmatrix}
\begin{pmatrix}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\
\beta_1 & \beta_2 & \beta_3 & \beta_4 \\
\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
\delta_1 & \delta_2 & \delta_3 & \delta_4
\end{pmatrix} =
\begin{pmatrix}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\
\beta_1 & \beta_2 & \beta_3 & \beta_4 \\
\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
\delta_1 & \delta_2 & \delta_3 & \delta_4
\end{pmatrix} = 1
\quad (1.12)
\]

Thus the commutation relations in a simple way define \( T^{-1} \) by the coefficients in \( T \). This property is the crucial point in this method and makes the diagonalization of \( H \) easy. We also note that \( T^{-1} \neq T^+ \) indicates that the transformation is non-unitary. From (1.7) we obtain \( H T = (T^+)^{-1} E \) or, explicitly,

\[
\begin{pmatrix}
A^a_q & B^k_q & C^k_q & D^k_q \\
B^k_q & A^a_{-q} & D^k_{-q} & C^k_{-q} \\
C^k_q & D^k_{-q} & A^b_q & B^k_q \\
D^k_q & C^k_{-q} & B^k_q & A^b_{-q}
\end{pmatrix}
\begin{pmatrix}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\
\beta_1 & \beta_2 & \beta_3 & \beta_4 \\
\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
\delta_1 & \delta_2 & \delta_3 & \delta_4
\end{pmatrix} =
\begin{pmatrix}
\alpha_1 & \alpha_2 & \alpha_3 & \alpha_4 \\
\beta_1 & \beta_2 & \beta_3 & \beta_4 \\
\gamma_1 & \gamma_2 & \gamma_3 & \gamma_4 \\
\delta_1 & \delta_2 & \delta_3 & \delta_4
\end{pmatrix} = E^f_q \quad (1.13)
\]
We notice that we can change signs in part of a column as follows:

\[
\begin{pmatrix}
\alpha \\
-\beta \\
\gamma \\
-\delta \\
\end{pmatrix} =
\begin{pmatrix}
1 & -1 \\
1 & -1 \\
& & 1 \\
& & & 1 \\
\end{pmatrix}
\begin{pmatrix}
\alpha \\
\beta \\
\gamma \\
\delta \\
\end{pmatrix}.
\] (1.14)

So for every column vector \( u_i \) of \( T \), (1.13) can be written as

\[
H \ u_i = \lambda_i \ B \ u_i \ ,
\] (1.15)

where \( B \) is the 4 x 4 matrix in (1.14)

\[
\lambda_1 = E^f_q, \ -\lambda_2 = E^f_{-q}, \ \lambda_3 = E^g_q, \ \text{and} \ -\lambda_4 = E^g_{-q}
\]

\( \lambda_i \) is the \( i \)th root of the determinant equation

\[
\det(H - \lambda B) = \left|
\begin{array}{cccc}
(A^a_q - \lambda) & B^a_k & C^k & D^k \\
B^a_q & (A^a_{-q} + \lambda) & D_{-q} & C_{-q} \\
C_q & D^k_{-q} & (A^b_q - \lambda) & B^b_k \\
D_q & C^k_{-q} & B^b_q & (A^b_{-q} + \lambda)
\end{array}
\right|
\] (1.16)

\[
= \lambda^4 + K_3 \lambda^3 + K_2 \lambda^2 + K_1 \lambda + K_0 = 0 .
\]

We are here only interested in the case where the energy is an even function of \( q \). In that case (1.16) is reduced to a second-order equation in \( \lambda^2 \).

Therefore we look for the cases where \( K_3 \) and \( K_1 \) vanish, \( ^* \)

\[
K_3 = A^a_{-q} - A^a_q + A^b_{-q} - A^b_q = 0 \ \text{for} \ A^a_q, b = A^a_{-q} . \] (1.17)

\( ^* \) The last condition in (1.17) is not the only possibility for making \( K_3 \) equal to zero; but it is the only one which does not impose restrictions between systems "a" and "b".
We then obtain the following condition for the other coefficients;

\[ K_1 = (|C_{-q}|^2 - |C_q|^2)(A_{q}^{a} + A_{q}^{b}) + (|D_{-q}|^2 - |D_q|^2)(A_{q}^{b} - A_{q}^{a}) \]

\[ + 2 \text{Re} \left[ B_{q}^{a} (C_{q} D_{-q} - C_{-q} D_{q}) + B_{q}^{b} (C_{q} D_{q} - C_{-q} D_{-q}) \right] = 0. \] 

(1.18)

When (1.17) and (1.18) are fulfilled, the solution to (1.16) has the form

\[ (\mathbf{w}_{q}^{f} \mathbf{g})^2 = (\mathbf{E}_{q}^{f} \mathbf{g})^2 = R^2 + \mathbf{S}^2 ; \] 

(1.19)

R and S are easily obtained from (1.16).

We shall here only give the explicit expression for a particular case.

Consider two equivalent systems in which the coefficients fulfil the conditions

\[ A_{q}^{a} = A_{q}^{b} = A_{q} = A_{-q} \quad \text{and} \quad B_{q}^{a} = B_{q}^{b} = B_{q} \quad \text{and} \quad C_{q} = C_{-q} \]. 

(1.20)

Then (1.17) and (1.18) are fulfilled with no conditions imposed on \( D_q \), and we have

\[ R = A_{q}^2 - |B_{q}|^2 + |C_{q}|^2 - \frac{|D_{q}|^2 + |D_{-q}|^2}{2} \] 

(1.21)

\[ S = 2|A_{q} C_{q} - B_{q}^{D} D_{q}|^2 + 2|A_{q} C_{-q} - B_{q}^{D} D_{-q}|^2 

- |B_{q}^{D} D_{q} - B_{q}^{D} D_{-q}|^2 - |C_{q} D_{-q} - C_{q}^D D_{q}|^2 + \frac{1}{4} \left[ |D_{q}|^2 - |D_{-q}|^2 \right]^2 \]

For \( D_q = D_{-q} = 0 \), (1.19) is reduced to

\[ (\mathbf{w}_{q}^{f} \mathbf{g})^2 = (A_{q}^2 + |C_{q}|^2) - |B_{q}|^2 . \] 

(1.22)

In the following we shall present a procedure for finding the coefficients of the transformation matrix \( \mathbf{T} \).
2. Method of Finding the Coefficients of the Transformation Matrix $T$

In the general case the problem of solving the equations (1.15) is troublesome. For some special cases the solution is given in many papers. The method described below, which is a kind of "step-transformation method", can be applied to a more general Hamiltonian, including that in which the absolute values of the coefficients $D_q$ and $D_{-q}$ are not equal. The idea is to write the $T$ matrix as a product of simpler matrices (four in the cases considered below) which describe simpler transformations. We apply this method to three cases, assuming such properties of the coefficients of the Hamiltonian (1.1) that the conditions (1.17), (1.18) and those mentioned just below (1.2) are fulfilled.

In all three cases we therefore assume $A_q^i = A_{-q}^i$ and real, and $B_q^i = B_{-q}^i$ ($i = a, b$). Besides, in particular cases the coefficients fulfill the following conditions:

1st case: $B_q^i$ arbitrary, $C_q = C_{-q}$, $D_q = D_{-q}$;

2nd case: $B_q^i$ real, $C_q = C_{-q}^K$, $D_q = D_{-q}^K$;

3rd case: $A^a_q = A^b_q$, $B^a_q = B^b_q$, $C_q = C_{-q}^K$, $D_q$ arbitrary.

\[
\begin{pmatrix}
p_1 & p_2 & 0 & 0 \\
p_3 & p_4 & 0 & 0 \\
p_5 & p_6 & 0 & 0 \\
p_7 & p_8 & 0 & 0
\end{pmatrix} \cdot \begin{pmatrix}
r_1 & 0 & 0 & r_2 \\
r_3 & r_4 & 0 & 0 \\
r_5 & r_6 & 0 & 0 \\
r_7 & 0 & 0 & r_8
\end{pmatrix} \cdot \begin{pmatrix}
1 & 0 & s_2 & 0 \\
0 & 1 & 0 & s_4 \\
0 & 0 & 1 & s_6 \\
0 & 0 & 0 & 1
\end{pmatrix} \cdot \begin{pmatrix}
t_1 & t_2 & 0 & 0 \\
t_3 & t_4 & 0 & 0 \\
t_5 & t_6 & 0 & 0 \\
t_7 & t_8 & 0 & 0
\end{pmatrix} = T_{II} \cdot T_{III} \cdot T_{IV} \cdot (2.1)
\]

\[^1\text{This is the case in a spin-wave treatment for instance of a spin system of hcp structure for which the Hamiltonian contains dipole-dipole or quadropole-quadropole interaction terms.}\]
2.1. First Case

In the first case the diagonalization is performed in the four steps given explicitly below.

We shall use the following notations (where it is not misleading, we omit the index q):

\[ A^a_q = A_1 \; ; \; \quad B^a_q = B_1 = |B_1| e^{i\varphi} \; ; \quad K_1^2 = A_1^2 - |B_1|^2 \; ; \]

\[ A^b_q = A_2 \; ; \; \quad B^b_q = B_2 = |B_2| e^{i\psi} \; ; \quad K_2^2 = A_2^2 - |B_2|^2 \; \tag{2.2} \]

(we here assume \( |B| < |A| \), which is usually the case),

and for the matrix coefficients:

\[ p_n = |p_n| e^{i\pi n} ; \quad r_n = |r_n| e^{i\sigma n} ; \quad s_n = |s_n| e^{i\varphi n} ; \quad t_n = |t_n| e^{i\tau n} ; \]

\[ (n = 1 \ldots 8) \; . \]

2.1.1. The first step transformation described by matrix \( T_I \)
transforms \( H \) (see (1.4) and (1.5)) into a similar expression with new coefficients \( A^i_{+q} \), \( B^i_{+q} \), \( C^i_{+q} \), \( D^i_{+q} \). Demanding that the transformation preserves commutation relations and gives \( B^i_{+q} = 0 \), we obtain the following values for \( p_n \):

\[
T_I = \begin{pmatrix}
  p_1 & p_2 & 0 & 0 \\
  p_3 & p_4 & 0 & 0 \\
  0 & 0 & p_5 & p_6 \\
  0 & 0 & p_7 & p_8
\end{pmatrix}
\]
A_1 + K_1 e^{i\pi_1} \quad \quad p_2 = \sqrt{\frac{A_1 - K_1}{2K_1}} e^{i\pi_2}

p_3 = -|p_2| e^{i\pi_1} \quad p_4 = -|p_1| e^{i\pi_2}

p_5 = \sqrt{\frac{A_2 + K_2}{2K_2}} e^{i\pi_5} \quad p_6 = \sqrt{\frac{A_2 - K_2}{2K_2}} e^{i\pi_6}

p_7 = -|p_6| e^{i\pi_5} \quad p_8 = -|p_5| e^{i\pi_6}

\pi_1, \pi_2, \pi_5, \pi_6, \text{ are arbitrary phase parameters.} \quad (2.3)

It turns out that

A_+^a = K_1; \quad A_+^b = K_2;

C_{q|l} = e^{i(\pi_1 - \pi_5)} e^{i\varphi} \left\{ C_q |p_1| |p_5| e^{-i\varphi} + C_{-q} |p_2| |p_6| e^{-i\varphi}
- D_q |p_1| |p_6| e^{-i(\varphi + \psi)} - D_{-q} |p_2| |p_5| \right\};

C_{-q|l} = e^{i(\pi_6 - \pi_2)} e^{i\varphi} \left\{ C_{-q} |p_1| |p_5| e^{-i\varphi} + C_q |p_2| |p_6| e^{-i\varphi}
- D_{-q} |p_1| |p_6| e^{-i(\varphi + \psi)} - D_q |p_2| |p_5| \right\};

(2.4)
\[
D_{q1} = e^{i(\pi_1 - \pi_6)} e^{i\varphi} \left\{ C_q |p_1| |p_6| e^{-i\varphi} + C_{-q}^K |p_2| |p_5| e^{-i\psi} - D_q |p_1| |p_5| e^{-i(\varphi + \psi)} - D_{-q}^K |p_2| |p_6| \right\};
\]

\[
D_{-q1} = e^{i(\pi_5 - \pi_2)} e^{i\psi} \left\{ C_{-q} |p_1| |p_6| e^{-i\varphi} + C_q^K |p_2| |p_5| e^{-i\psi} - D_{-q} |p_1| |p_5| e^{-i(\varphi + \psi)} - D_q^K |p_2| |p_6| \right\}.
\]

(2.5)

---

We see that the conditions $C_q = C_{-q}$, $D_q = D_{-q}$ give $|C_{q1}| = |C_{-q1}|$ and $|D_{q1}| = |D_{-q1}|$ for arbitrary $B_i^q$.

In the second case, where we assume $C_q = C_{-q}^K$, $D_q = D_{-q}^K$, it is necessary to assume also $B_i^q$ real in order to get $|C_{q1}| = |C_{-q1}|$, $|D_{q1}| = |D_{-q1}|$. These conditions are required in order that the next step transformation may be performed.

2.1.2 In the second step transformation we shall use the following notations:

\[
C_{-q1} = M_{-q1}; \quad D_{-q1} = N_{+q1}; \quad |M_q| = |M_{-q1}|; \quad |N_q| = |N_{-q1}| \quad ; (2.6)
\]

\[
Q_1 = \frac{K_1 - K_2}{2} + \sqrt{\left(\frac{K_1 + K_2}{2}\right)^2 - |N_q|^2};
\]

(2.7)

\[
Q_2 = \frac{K_2 - K_1}{2} + \sqrt{\left(\frac{K_1 + K_2}{2}\right)^2 - |N_{-q1}|^2}.
\]

One can easily check that $K_1 - Q_1 = K_2 - Q_2$ and

\[
|N_q|^2 = |N_{-q1}|^2 = (K_1 - Q_1)(K_1 + Q_2).
\]
This is the transformation described by matrix $T_{\Pi}$. It transforms the considered part of the Hamiltonian into a new one with the coefficients $A^i_{-qll}, B^i_{-qll}, C^i_{-qll}, D^i_{-qll}$.

Demanding that the transformation preserves commutation relations and gives $D^+_q = 0$, we obtain the following values for the coefficients $r_n$:

$$
\begin{align*}
T_{\Pi} &= \begin{pmatrix}
 r_1 & 0 & 0 & r_2 \\
 0 & r_3 & r_4 & 0 \\
 0 & r_5 & r_6 & 0 \\
 r_7 & 0 & 0 & r_8
\end{pmatrix} \\

r_1 &= \sqrt{\frac{K_1 + Q_2}{Q_1 + Q_2}} e^{i \xi_1} \\
r_2 &= \sqrt{\frac{K_1 - Q_1}{Q_1 + Q_2}} e^{i \xi_2} \\
r_3 &= |r_1| e^{i \xi_3} \\
r_4 &= |r_2| e^{i \xi_4} \\
r_5 &= -|r_2| \frac{N^q}{|N^q|} e^{i \xi_3} \\
r_6 &= -|r_1| \frac{N^q}{|N^q|} e^{i \xi_4} \\
r_7 &= -|r_2| \frac{N^q}{|N^q|} e^{i \xi_1} \\
r_8 &= -|r_1| \frac{N^q}{|N^q|} e^{i \xi_2}
\end{align*}
$$

(2.8)

$\xi_1, \xi_2, \xi_3, \xi_4$ are arbitrary phase parameters.
It turns out that

\[ A^a_{-qll} = Q_1 \quad ; \quad A^b_{-qll} = Q_2 \]  
(2.9)

\[ B^a_{-qll} = -\frac{|r_1| |r_2|}{|N_q|} \left\{ M_q N_{-q} + M_{-q} N_q \right\} e^{i(\delta_1 - \delta_3)} \]  
(2.10)

\[ B^b_{-qll} = -\frac{|r_1| |r_2|}{|N_q|} \left\{ M^*_q N^*_{-q} + M^*_{-q} N^*_q \right\} e^{-i(\delta_2 - \delta_4)} \]

\[ C_{qll} = \frac{-1}{|N_q|} \left\{ |r_1|^2 M_q N_{-q} + |r_2|^2 M_{-q} N_q \right\} e^{i(\delta_1 - \delta_3)} \]  
(2.11)

\[ C^\kappa_{-qll} = \frac{-1}{|N_q|} \left\{ |r_2|^2 M^*_q N^*_{-q} + |r_1|^2 M^*_{-q} N^*_q \right\} e^{-i(\delta_2 - \delta_4)} \]

If we assume the following relation between the arbitrary phase factors:

\[ e^{i(\delta_1 - \delta_3)} = e^{-i(\delta_2 - \delta_4)} \frac{M^*_q N^*_{-q}}{M_q N_{-q}} \], and use (2.6), we obtain the relation

\[ B^a_{qll} = B^b_{qll} \quad \text{and at the same time} \quad C_{qll} = C^\kappa_{-qll} \]  
(2.12)

2.1.3. In the third step transformation we shall use the following notations:

\[ C_{qll} = P_q \quad ; \quad P_q = P^\kappa_{-q} \quad ; \quad B^a_{qll} = B^b_{qll} = U_q \]  
(2.13)

\[ W_1 = \frac{Q_1 + Q_2}{2} + \sqrt{\left(\frac{Q_1 - Q_2}{2}\right)^2 + |P_q|^2} \]  
(2.14)

\[ W_2 = \frac{Q_1 + Q_2}{2} - \sqrt{\left(\frac{Q_1 - Q_2}{2}\right)^2 + |P_{-q}|^2} \]
The third step transformation described by the matrix $T_{III}$ transforms the considered part of the Hamiltonian into a new one with the coefficients $A_{qIII}^i$, $B_{qIII}^i$, $C_{qIII}$, $D_{qIII}$.

Demanding that the transformation preserves commutation relations and gives $C_{qIII}$ = 0, we obtain the following values for the coefficients $s_n$:

$$
T_{III} = \begin{pmatrix}
s_1 & 0 & s_2 & 0 \\
0 & s_3 & 0 & s_4 \\
s_5 & 0 & s_6 & 0 \\
0 & s_7 & 0 & s_8
\end{pmatrix}
$$

\[
s_1 = \sqrt{\frac{Q_1 - W_2}{W_1 - W_2}} \ e^{id_1} \\
s_2 = \sqrt{\frac{W_1 - Q_1}{W_1 - W_2}} \ e^{id_2} \\
s_3 = |s_1| \ e^{id_3} \\
s_4 = |s_2| \ e^{id_4} \\
s_5 = |s_2| \ \frac{P_q}{|P_q|} \ e^{id_1} \\
s_6 = -|s_1| \ \frac{P_q}{|P_q|} \ e^{id_2} \\
s_7 = |s_2| \ \frac{P_q}{|P_q|} \ e^{id_3} \\
s_8 = -|s_1| \ \frac{P_q}{|P_q|} \ e^{id_4}
\]

(2.15)

$d_1$, $d_2$, $d_3$, $d_4$ are arbitrary phase parameters.

It turns out that

$$
A_{qIII}^a = W_1 ; \quad A_{qIII}^b = W_2 ;
$$

$$
B_{qIII}^a = B_{qIII}^b = U_q e^{i(d_1 - d_3)} \quad \text{if we assume} \quad e^{i(d_2 - d_4)} = e^{i(d_1 - d_3)};
$$

(2.16)
D_+T = 0 ; this follows from the relations (2.12).

So we see that after performing the three above step transformations we get a transformed Hamiltonian with only A and B coefficients different from zero. Therefore, to obtain a completely diagonalized form we have to perform a fourth step transformation of the same type as the first.

2.1.4. In the fourth step transformation we shall use the following notations:

\[ E_1 = \sqrt{W_1^2 - |U|^2} \]
\[ E_2 = \sqrt{W_2^2 - |U|^2} \]
\[ U = \frac{i(d_1 - d_3)}{2} = X. \]

(2.17)

Demanding that the transformation with matrix \( T_{IV} \) preserves commutation relations and gives \( B^{il}_{qIV} = 0 \), we obtain the following values for the coefficients \( t_n \):

\[
T_{IV} = \begin{pmatrix}
    t_1 & t_2 & 0 & 0 \\
    t_3 & t_4 & 0 & 0 \\
    0 & 0 & t_5 & t_6 \\
    0 & 0 & t_7 & t_8
\end{pmatrix}
\]

\[
t_1 = \sqrt{\frac{W_1 + E_1}{2E_1}} e^{i\tau_1} \\
t_2 = \sqrt{\frac{W_1 - E_1}{2E_1}} e^{i\tau_2} \\
t_3 = -|t_2| \frac{X}{|X|} e^{i\tau_1} \\
t_4 = -|t_1| \frac{X}{|X|} e^{i\tau_2} \\
t_5 = \sqrt{\frac{W_2 + E_2}{2E_2}} e^{i\tau_5} \\
t_6 = \sqrt{\frac{W_2 - E_2}{2E_2}} e^{i\tau_6} \\
t_7 = -|t_8| \frac{X}{|X|} e^{i\tau_5} \\
t_8 = -|t_5| \frac{X}{|X|} e^{i\tau_6}
\]

(2.18)
The phase parameters \( \tau_1, \tau_2, \tau_5, \tau_6 \) are arbitrary phase parameters.

It turns out that \( A^a_{+q} = E_1 \), \( A^b_{+q} = E_2 \), and all other coefficients are equal to zero.

### 2.2. Second Case

In the second case, where we assume \( H_i \) real, \( C_q = C^x_{-q} \), \( D_q = D^x_{-q} \), the procedure is completely similar to that for the first case (see the remark just below (2.5)).

In both cases matrix \( T \) is only determined within four arbitrary phase factors, one for each column. We can use this arbitrariness if we want the coefficients of the matrix \( T \) to fulfill the conditions \( \gamma_i(-q) = \gamma_i(q) \).

### 2.3. Third Case

In the third case \( (A^a_q = A^b_q, B^a_q = B^b_q, C_q = C^x_{-q}, D_q \) arbitrary) we have generally \( |D_q| \neq |D_{-q}| \), so we cannot follow the procedure of the first and second cases because now \( |M_q| \neq |M_{-q}| \) and \( |N_q| \neq |N_{-q}| \).

#### 2.3.1. Therefore we change the first step transformation, using to describe it matrix \( T_1' \) of the shape

\[
T_1' = \begin{pmatrix}
  p_1' & p_2' & 0 & 0 \\
  0 & 0 & p_3' & p_4' \\
  0 & 0 & p_5' & p_6' \\
  p_7' & p_8' & 0 & 0
\end{pmatrix}
\]  

(2.19)

We shall use the following notations:

\[
A^a_q = A^b_q = A ; \quad B^a_q = B^b_q = B
\]  

(2.20)

\[
K_1 = \sqrt{A^2 - |D_q|^2} \quad ; \quad K_2 = \sqrt{A^2 - |D_{-q}|^2}
\]  

(2.21)
Performing this transformation, we obtain new coefficients $A_{\pm q}^i$, $B_{\pm q}^i$, $C_{\pm q}$, $D_{\pm q}$. Demanding that the transformation preserves commutation relations and gives $B_{\pm q}^i = 0$, we obtain the following values for the coefficients $p_n'$:

\[
\begin{align*}
  p_1' &= \sqrt{\frac{A + K_1}{2 K_1}} e^{i \pi_1} \\
  p_2' &= \sqrt{\frac{A - K_1}{2 K_1}} e^{i \pi_2} \\
  p_3' &= \sqrt{\frac{A - K_2}{2 K_2}} e^{i \pi_3} \\
  p_4' &= \sqrt{\frac{A + K_2}{2 K_2}} e^{i \pi_4} \\
  p_5' &= -|p_4'| \frac{D^*}{|D^* - q|} e^{i \pi_3} \\
  p_6' &= -|p_3'| \frac{D^*}{|D^* - q|} e^{i \pi_4} \\
  p_7' &= -|p_2'| \frac{D^*}{|D^* - q|} e^{i \pi_1} \\
  p_8' &= -|p_1'| \frac{D^*}{|D^* - q|} e^{i \pi_2}
\end{align*}
\]

(2.22)

$\pi_1$, $\pi_2$, $\pi_3$, $\pi_4$ are arbitrary phase parameters.

It turns out that

\[
A_{\pm q}^a = K_1; \quad A_{\pm q}^b = K_2
\]

(2.23)
\[
C_{ql} = e^{i(\pi_1 - \pi_2)} \left\{- C_q |p'_1| |p'_4| \frac{D_{-q}}{|D_{-q}|} - C_q |p'_2| |p'_3| \frac{D_{q}}{|D_{q}|} + B |p'_1| |p'_3| + B^x |p'_2| |p'_4| \frac{D_{-q} D_{q}}{|D_{-q}| |D_{q}|} \right\};
\]

\[
C_{-ql} = e^{i(\pi_1 - \pi_3)} \left\{- C_q |p'_1| |p'_4| \frac{D_{q}}{|D_{q}|} - C_q |p'_2| |p'_3| \frac{D^x_{-q}}{|D^x_{-q}|} + B^x |p'_2| |p'_4| \frac{D^x_{-q} D^x_{q}}{|D^x_{-q}| |D^x_{q}|} + B |p'_1| |p'_3| \frac{D^x_{-q} D^x_{q}}{|D^x_{-q}| |D^x_{q}|} \right\};
\]

\[
D_{ql} = e^{i(\pi_1 - \pi_4)} \left\{- C_q |p'_1| |p'_3| \frac{D_{q}}{|D_{q}|} - C_q |p'_2| |p'_4| \frac{D_{q}}{|D_{q}|} + B |p'_1| |p'_4| + B^x |p'_2| |p'_3| \frac{D_{q} D_{-q}}{|D_{q}| |D_{q}|} \right\};
\]

(2.24)

We can get \(C_{ql} = C_{-ql}\) if we assume \(e^{i(\pi_1 - \pi_3)} = e^{i(\pi_4 - \pi_2)}\) \(\frac{D^x_{-q} D^x_{q}}{|D^x_{-q}| |D^x_{q}|}\)

(2.25)

\(D_{ql} = D_{-ql}\) if condition (2.25) is fulfilled.

Putting again \(C_{ql} = M_q\), \(D_{ql} = N_q\), we have \(|M_q| = |M_{-q}|, |N_q| = |N_{-q}|\).

and we can perform second, third and fourth step transformations as before.

Also as before, matrix \(T\) will be determined within four arbitrary phase factors, one for each column.
3. Conclusion

We have shown that a bilinear Bose Hamiltonian can be diagonalized in a simple way by a method analogous with that used for the diagonalization of a quadratic form of c-number variables. The fact that we have been dealing with Bose operators reveals itself in the matrix $B$ (1.14 and 1.15), which in the case of c-numbers is the unit matrix. The Bose commutation relations thus introduce the strain (1.12) on the coefficients in the transformation matrix $T$

$$T_{ij} = (-)^{i+j} T_{ji}^k.$$  \(3.1\)

It should be noted that the strain condition (or the matrix $B$) is dependent not only on the (BCR), but also on the sequence chosen of the operators in the quadratic form (1.4).

In section 2 it has been shown how it is possible to obtain the coefficients $T_{ij}$, subjected to the strain (3.1) when certain relations are fulfilled between the matrix elements of the hermetian matrix, which is to be made diagonal. The strain (3.1) is clearly independent of the following changes in the operator sequence in (1.4): $a_q \leftrightarrow b_q$ and/or $a_{-q} \leftrightarrow b_{-q}$. The result of the step transformations in section 2 can thus also be applied to other cases of interrelations between $A_q^i$, $B_q^1$, $C_q^i$, and $D_q$ than those quoted in cases I to III. As an example of this it is easily checked that case III is comprised by case I when the rearrangement $a_q \leftrightarrow b_q$, $a_{-q}$ and $b_{-q}$ unchanged, is made. Finally it should be mentioned that the method used in sec. 1 can be applied to any quadratic form of operators for which the commutation relations are equal to c-numbers$^4$). In general the matrix $B$ will not be diagonal.

Acknowledgement

We should like to thank Mr. P. Laut for numerous discussions.
Appendix 1. Calculation of Energies in the Third Case

We can easily calculate the energies $E_1$, $E_2$ for instance in the third case. We start from the formula (2.17) with $M_q$, $N_q$ given by (2.24), (2.26) and (2.6):

$$E_1^2 = W_1^2 - |U|^2 = \left(\frac{Q_1 + Q_2}{2}\right)^2 + \left(\frac{Q_1 - Q_2}{2}\right)^2 + |P|^2 - |U|^2$$

$$+ \sqrt{\left(\frac{Q_1^2 - Q_2^2}{4}\right)^2 + |P|^2 \left(Q_1^2 - Q_2^2\right)^2}$$

$$= R + \sqrt{S} \quad \text{(compare with (1.19))},$$

where $|P|^2 = |M|^2 \frac{(K_1 + K_2)^2}{(Q_1 + Q_2)^2}$ and $|U|^2 = \frac{4 |M|^2 |N|^2}{(Q_1 + Q_2)^2}$.

$$R = \frac{1}{2} Q_1^2 + \frac{1}{2} Q_2^2 + |P|^2 - |U|^2 = \frac{1}{2} (Q_1^2 + Q_2^2) + |M|^2$$

$$= \left(\frac{K_1 - K_2}{2}\right)^2 + \left(\frac{K_1 + K_2}{2}\right)^2 - |N|^2 + |M|^2 = A^2 - \frac{|D_q|^2 + |D_q|^2 - |N|^2 - |M|^2}{2}.$$

$$S = \left[\frac{Q_1^2 - Q_2^2}{4}\right]^2 + |M|^2 (K_1 + K_2)^2 = \frac{1}{4} \left[K_1^2 - K_2^2\right]^2 -(K_1 - K_2)^2 |N|^2 + (K_1 + K_2)^2 |M|^2$$

$$= \frac{1}{4} \left(|D_q|^2 - |D_q|^2\right)^2 + (K_1 + K_2)^2 (|M|^2 - |N|^2) + 2 K_1 K_2 (|M|^2 + |N|^2).$$

From the definitions of $M_q$ and $N_q$ we obtain (putting $C_q = C$)
\[ |M|^2 = \frac{1}{4K_1K_2} \left\{ 2A^2(|C|^2 + |B|^2) + 2K_1K_2(|C|^2 - |B|^2) + 2ReC^2D_qD^{\#}_{-q} \\
+ 2ReB^2D^{\#}_{q}D^{\#}_{-q} \\
- 4ReABCD^{\#}_{-q} \\
- 4ReAB^*CD_q \right\}; \]

\[ |N|^2 = \frac{1}{4K_1K_2} \left\{ 2A^2(|C|^2 + |B|^2) + 2K_1K_2(|B|^2 - |C|^2) + 2ReC^2D_qD^{\#}_{-q} \\
+ 2ReB^2D^{\#}_{q}D^{\#}_{-q} \\
- 4ReABCD^{\#}_{-q} \\
- 4ReAB^*CD_q \right\}; \]

Putting these expressions for \( |M|^2 \) and \( |N|^2 \) into \( R \) and \( S \), we obtain formula (1.22).
Appendix 2. Explicit Calculation of the Matrix \( T \) for a Special Case

\[
A^a_q = A^b_q = A; \quad B^a_q = B^b_q = B \quad \text{(not necessarily real)};
\]
\[
C^q = C^{-q}; \quad D^q = D^{-q} = 0.
\]

This example is comprised by case III. Let us make the additional assumption that \( A > 0 \) (if not, we could always write \( H = - (-H) \) and diagonalize \( -H \)) and use the notation \( B = |B| e^{i\Phi}, \ C_q = |C_q| e^{i\Phi}. \) All formulae introduced in the description of the four step transformations will now be very simple. Starting at section 2.3, we obtain

\[
K_1 = K_2 = A
\]
\[
N_q = N^{-q} = |B| e^{i(\pi_1 - \pi_4)} e^{i\Phi}
\]
\[
M_q = M^{-q} = |C| e^{i(\pi_1 - \pi_3)} e^{i\Phi'} = |C| e^{i(\pi_4 - \pi_2)} e^{i\Phi'}
\]
\[
Q_1 = Q_2 = \sqrt{A^2 - |B|^2} = Q
\]
\[
P_q = N^{-q} = \frac{A|C|}{Q} e^{i(\xi_1 - \xi_4)} e^{i(\pi_1 - \pi_2)} e^{i\Phi} e^{i\Phi'} = P
\]
\[
X = 2 |B| |C| e^{i(\xi_1 - \xi_3)} e^{i(\xi_1 - \xi_3)} e^{i(\pi_1 - \pi_2)} e^{i\Phi} e^{i\Phi'}
\]
\[
W_1 - W_2 = 2(W_1 - Q) = 2(Q - W_2) = 2 |P|
\]
\[
E_1^2 = (A + |C|)^2 - |B|^2 \quad \quad E_2^2 = (A - |C|)^2 - |B|^2.
\]

The relations (2.25), (2.16), (2.12) between the otherwise arbitrary phase factors \( \pi_n, \xi_n, \delta_n \) are now
\[
\begin{pmatrix}
  i(\pi_1 - \pi_2) & i(\pi_4 - \pi_2) \\
  e & e \\
  e & e \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
  i(\sigma_2 - \sigma_4) & i(\sigma_1 - \sigma_3) \\
  e & e \\
  e & e \\
\end{pmatrix}
\]

\[
\begin{pmatrix}
  i(\xi_1 - \xi_3) & -i(\xi_2 - \xi_4) & 2i(\pi_2 - \pi_1) & -2i(\varphi + \varphi') \\
  e & e & e & e \\
\end{pmatrix}
\]

The matrices of the four step transformations are then

\[
T_1 = \begin{pmatrix}
  i\pi_1 & 0 & 0 & 0 \\
  e & 0 & 0 & i\pi_4 \\
  0 & 0 & 0 & e \\
  0 & 0 & -i\pi_3 & 0 \\
  0 & -e & 0 & 0 \\
\end{pmatrix}
\]

\[
T_{\text{III}} = \frac{1}{\sqrt{2}} \begin{pmatrix}
  i\sigma_1 & 0 & i\sigma_2 & 0 \\
  e & 0 & i\sigma_3 & 0 \\
  0 & i\sigma_4 & e & 0 \\
  \frac{P}{|P|} e^{i\sigma_1} & 0 & -\frac{P}{|P|} e^{i\sigma_2} & 0 \\
  0 & \frac{P}{|P|} e^{i\sigma_3} & 0 & -\frac{P}{|P|} e^{i\sigma_4} \\
\end{pmatrix}
\]
Multiplying the four matrices by one another, we obtain matrix $T$ with the following elements:

**First column:**

$$a_1 = \frac{1}{\sqrt{8Q E_1}} e^{i\left(\frac{\pi_1 + g_1 + \delta'_1 + \tau_1}{2}\right)} \left\{ \sqrt{(A + Q)(W_1 + E_1)} - \sqrt{(A - Q)(W_1 - E_1)} \right\}$$

Let us denote the expression in the braces as $L$; then

$$L^2 = 2Q(A + |C| + E_1).$$

If $|B|$ is small, which is usually the case, $L > 0$ and $a_1$ becomes

$$a_1 = \frac{1}{2\sqrt{E_1}} e^{i\left(\frac{\pi_1 + g_1 + \delta'_1 + \tau_1}{2}\right)} \sqrt{A + |C| + E_1}.$$

$$\beta_2^x = \frac{1}{\sqrt{8QE_1}} e^{i\phi} e^{i\left(\frac{\pi_1 + g_1 + \delta'_1 + \tau_1}{2}\right)} \left\{ -\sqrt{(A-Q)(W_1+E_1)} + \sqrt{(A+Q)(W_1-E_1)} \right\}.$$

Denoting the expression in the braces as $L'$, we obtain

$$(L')^2 = 2Q(A + |C| - E_1).$$

It turns out that, for small $|B|$, $L' < 0$ and $\beta_2^x$ becomes

$$\beta_2^x = \frac{-1}{2\sqrt{E_1}} \frac{B}{|B|} e^{i\left(\frac{\pi_1 + g_1 + \delta'_1 + \tau_1}{2}\right)} \sqrt{A + |C| - E_1}.$$

Similarly we get

$$\gamma_1 = \frac{1}{2\sqrt{E_1}} \frac{C}{|C|} e^{i\left(\frac{\pi_1 + g_1 + \delta'_1 + \tau_1}{2}\right)} \sqrt{A + |C| + E_1}.$$

$$\delta_2^x = \frac{-1}{2\sqrt{E_1}} \frac{B}{|B|} \frac{C}{|C|} e^{i\left(\frac{\pi_1 + g_1 + \delta'_1 + \tau_1}{2}\right)} \sqrt{A + |C| - E_1}.$$
Second column:

\[ a_2 = \frac{-1}{2 \sqrt{E_1}} e^{i(n_1 + s_1 + d_1 + \tau_2) \sqrt{A + |C| - E_1}} \]

\[ \beta_1^x = \frac{1}{2 \sqrt{|E_1| |B|}} e^{i(n_1 + s_1 + d_1 + \tau_2) \sqrt{A + |C| + E_1}} \]

\[ \gamma_2 = \frac{C}{|C|} a_2 \]

\[ \delta_1^x = \frac{C}{|C|} \beta_1^x \]

Third column:

\[ a_3 = \frac{1}{2 \sqrt{E_2}} e^{i(n_1 + s_2 + d_2 + \tau_3) \sqrt{A + |C| + E_2}} \]

\[ \phi_4^x = \frac{-1}{2 \sqrt{E_2}} \frac{B}{|B|} e^{i(n_1 + s_1 + d_2 + \tau_3) \sqrt{A + |C| - E_2}} \]

\[ \gamma_3 = -\frac{C}{|C|} a_3 \]

\[ \delta_4^x = -\frac{C}{|C|} \beta_4^x \]

Fourth column:

\[ a_4 = \frac{1}{2 \sqrt{E_2}} e^{i(n_1 + s_2 + d_2 + \tau_6) \sqrt{A + |C| - E_2}} \]

\[ \beta_3^x = \frac{-1}{2 \sqrt{E_2}} \frac{B}{|B|} e^{i(n_1 + s_1 + d_2 + \tau_6) \sqrt{A + |C| + E_2}} \]
\[ \gamma_4 = -\frac{C}{|C|} a_4 \]

\[ \delta_3^1 = -\frac{C}{|C|} \beta_3^1 . \]

Putting the following values for the arbitrary phase factors:

\[ e^{i(\pi_1 + \phi_1 + d_1 + \tau_1)} = 1 , \quad e^{i(\pi_1 + \phi_1 + d_1 + \tau_2)} = \frac{E^x}{|B|} \]

\[ e^{i(\pi_1 + \phi_1 + d_2 + \tau_3)} = 1 , \quad e^{i(\pi_1 + \phi_1 + d_2 + \tau_6)} = -\frac{E^x}{|B|} . \]

we can, using the same notation as in ref. 2., write matrix \( T \) as

\[
T = \begin{pmatrix}
p_o - m_o & p_a - m_a \\
-m_o & p_o - m_a & p_a \\
cp_o - cm_o & -cp_a & cm_o \\
cm_o & cp_o & cm_a - cp_a
\end{pmatrix}
\]

where

\[
m_{o,a} = \frac{B}{|B|} \sqrt{\frac{E_{o,a}^2 + |B|^2}{4 E_{o,a}}} - E_{o,a}
\]

\[
p_{o,a} = \sqrt{\frac{E_{o,a}^2 + |B|^2 + E_{o,a}}{4 E_{o,a}}}
\]

\[
c = \frac{C}{|C|} .
\]
$E_0, a$ here stand for $E_{1,2}$ and may denote the optical and the accoustical energy respectively. Note that

$$A + |C| = \sqrt{E_1^2 + |B|^2}$$

and

$$A - |C| = \sqrt{E_2^2 + |B|^2}$$
References


