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Cite as: Journal of Mathematical Physics **19**, 277 (1978); <https://doi.org/10.1063/1.523549>

Published Online: 11 August 2008

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# Diagonalization methods for the general bilinear Hamiltonian of an assembly of bosons

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(Received 27 June 1977)

The problem of the exact diagonalization of the Hamiltonian of an assembly of  $N$  bilinearly interacting bosons is discussed in what concerns the eigenvalues as well as for the expression of the new boson operators in terms of the old ones. The method is equivalent to the standard equation-of-motion approach, nevertheless sensibly more concise. Three sets of operational rules are indicated, and their use is exhibited in some examples. In some particular cases of practical importance (for example, when all the coefficients of the Hamiltonian are real), the research of the eigenvalues has been compacted as much as possible.

## 1. INTRODUCTION

It is well known from long date (at least from the date of Bogolyubov's paper<sup>1</sup> on superfluidity in 1947), that the Hamiltonian of an assembly of  $N$  bilinearly interacting bosons (or fermions) is susceptible of exact diagonalization, in terms of new noninteracting bosons (or fermions). The standard method used to perform such a diagonalization is the so-called "equation-of-motion approach," proposed by Bogolyubov and Tyablikov<sup>2-4</sup> in the years 1947-49 and by Bohm and Pines<sup>5</sup> in 1953. This approach is formally presented (see for example Refs. 6 and 7) and discussed<sup>8,9</sup> by several authors. It is equally useful for fermion problems<sup>10-13</sup> (see Refs. 14 and 15 for superconductivity) and boson problems<sup>1,16-18</sup> (phonon-phonon,<sup>16</sup> photon-optical phonon,<sup>16</sup> magnon-magnon,<sup>16,17</sup> phonon-pseudomagnon<sup>18</sup> interactions, etc.). Because of the wideness of the applications of this diagonalization problem, we thought it was worthwhile trying to put it in compact operational rules, and this is the purpose of the present work. However, only the boson case is extensively examined, as in the fermion case, the canonical transformation between old and new fermions is given by a unitary matrix with no further complications. This is not so for the boson case, where the canonical transformation is governed by a matrix related to a not necessarily positive metric, a fact which introduces a certain amount of "pathology" in the case.

In Sec. 2 we present the Hamiltonian we are going to deal with; in Sec. 3 the basic ideas of the diagonalization appear, which lead to the three sets of operational rules of Sec. 6; in Secs. 4 and 5 a particular canonical transformation and the treatment of particular Hamiltonians respectively appear; we conclude in Sec. 7 with a practical comparison between the three diagonalizing methods exposed in this paper; finally the Appendix treats the cases  $N=1, 2, 3$  ( $N=1$  corresponds to the historical form of Bogolyubov's transformation).

## 2. HAMILTONIAN

Let us consider an assembly of  $N$  bilinearly interacting bosons, which might be particles or quasiparticles. The most general<sup>19</sup> quadratic Hamiltonian (which doesn't need to conserve the number of bosons) might be written as follows:

$$H = \sum_{i=1}^N \sum_{j=1}^N \left( 2\omega_{ij} b_i^\dagger b_j + \nu_{ij}^1 b_i^\dagger b_j^\dagger + \nu_{ij}^2 b_i b_j \right), \quad (1)$$

where the factor 2 has been introduced for future use;  $\omega_{ij}$ ,  $\nu_{ij}^1$ , and  $\nu_{ij}^2$  are complex numbers, and the creation and annihilation operators satisfy

$$[b_i, b_j] = [b_i^\dagger, b_j^\dagger] = 0 \quad \forall (i, j), \quad (2a)$$

$$[b_i, b_j^\dagger] = \delta_{ij} \equiv \text{Kronecker's delta} \quad \forall (i, j). \quad (2b)$$

Our final purpose is of course to present this Hamiltonian in the form

$$H = \sum_{j=1}^N 2\Omega_j B_j^\dagger B_j, \quad (3)$$

where  $\Omega_j$  should be known real positive functions of the previous parameters, and the new boson operators are known linear combinations of the old ones.

Let us use the notation  $\omega$ ,  $\nu^1$ , and  $\nu^2$  for denoting the matrix  $\{\omega_{ij}\}$ ,  $\{\nu_{ij}^1\}$ , and  $\{\nu_{ij}^2\}$ , respectively. Because of commutation rules (2a) we may always consider  $\nu^1$  and  $\nu^2$  as symmetric matrices. Furthermore, hermiticity of  $H$  implies hermiticity of  $\omega$  as well as  $\nu^{2*} = \nu^1 \equiv \nu$ , where  $*$  denotes the complex conjugate. Hence (1) may be rewritten as follows:

$$H = \sum_{i,j} \{ \omega_{ij} b_i^\dagger b_j + \omega_{ij}^* b_i b_j^\dagger + \nu_{ij} b_i^\dagger b_j^\dagger + \nu_{ij}^* b_i b_i \}, \quad (1')$$

where  $\omega = \omega^*$  and  $\nu = \nu^T$  (+ and  $T$  denote the adjoint and the transposed matrix respectively.) Let us now introduce the nomenclature

$$|b\rangle \equiv \begin{bmatrix} b_1 \\ \vdots \\ b_N \\ b_1^\dagger \\ \vdots \\ b_N^\dagger \end{bmatrix}, \quad \langle b| \equiv |b\rangle^* = (b_1^*, \dots, b_N^*, b_1, \dots, b_N),$$

$$H \equiv \begin{bmatrix} \omega & \nu \\ \nu^* & \omega^* \end{bmatrix} \quad (H^* = H).$$

We note that if  $H$  conserves the number of  $b$  bosons,<sup>20</sup> then  $\nu=0$ . The Hamiltonian (1') and the commutation rules (2a), (2b) may be written as follows:

$$H = \langle b | H | b \rangle, \quad (1'')$$

$$|b\rangle\langle b| - (|b^*\rangle\langle b^*|)^T = J \equiv \begin{bmatrix} 1_N & 0_N \\ 0_N & -1_N \end{bmatrix}, \quad (2'')$$

where  $|\cdots\rangle\langle\cdots|$  means the matrix direct product, and  $1_N$  and  $0_N$  denote the  $N \times N$  unity and zero matrix respectively. We note that  $|b^*\rangle \neq |b\rangle^*$ .

### 3. DIAGONALIZING METHOD

Let us first of all state a basic property: The Hamiltonian given by (1') will be diagonal in  $b$ 's operators (this is to say  $\nu=0$  and  $\omega$  is diagonal) if and only if

$$[H, b_i] = -2\omega_i b_i \quad \forall i.$$

The proof is straightforward once we have remarked that in general

$$[H, b_i] = -2 \sum_j \{ \omega_{ij} b_j + \nu_{ij} b_{j1}^* \} \quad \forall i.$$

This is the property we shall use to find the new boson operators  $B$ 's which put  $H$  into diagonal form, this is to say

$$H = \langle B | H_D | B \rangle, \quad (3')$$

where

$$H_D \equiv \begin{bmatrix} \Omega & 0_N \\ 0_N & \Omega \end{bmatrix}$$

and

$$\Omega \equiv \begin{bmatrix} \Omega_1 & 0 & \dots & 0 \\ 0 & \Omega_2 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \dots & \Omega_N \end{bmatrix}.$$

To perform the diagonalization let us propose

$$\langle B | = \langle b | T \quad \text{and} \quad | B \rangle = T^* | b \rangle,$$

where  $T$  is a  $2N \times 2N$  matrix to be found. In order to have that  $B_j^*$  be the adjoint of  $B_j$ ,  $T$  must have a particular form:

$$T = \begin{bmatrix} T_1 & T_2 \\ T_2^* & T_1^* \end{bmatrix}. \quad (4)$$

As we want the  $B$ 's to be boson operators, they must also satisfy the commutation rules

$$|B\rangle\langle B| - (|B^*\rangle\langle B^*|)^T = J \quad (5)$$

which implies (once we have remarked that  $|B^*\rangle = T^* | b^* \rangle$ ) that

$$T^* J T J = 1_{2N} \quad \text{hence} \quad T^{-1} = J T^* J. \quad (5')$$

We see as a corollary that the modulus of the determinant of  $T$  equals one. It is also easily verified that the ensemble of the matrix  $T$  satisfying (4) and (5') constitutes a Lie group (in general non-Abelian). Relation

(5') may be written

$$T_1^* T_1 - T_2^T T_2^* = 1_N, \quad (5''a)$$

$$T_2^* T_1 - T_1^T T_2^* = 0_N. \quad (5''b)$$

To be sure that  $H$  is diagonal we impose

$$[H, B_j] = -2\Omega_j B_j \quad \forall j,$$

$$[H, B_j^*] = 2\Omega_j B_j^* \quad \forall j$$

or more compactly

$$[H, |B\rangle] = -2JH_D |B\rangle. \quad (6)$$

Taking into account that

$$\begin{aligned} [H, |B\rangle] &= [H, T^* | b \rangle] \\ &= T^* [H, | b \rangle] = -2T^* JH | b \rangle, \end{aligned}$$

relation (6) immediately implies that

$$T^* JH = JH_D T^*. \quad (6')$$

Hence

$$T^{-1} H J T = H_D J, \quad (6'')$$

where we have used relation (5'). And taking into account the particular form of  $T$ , (6'') may be rewritten as follows:

$$\begin{bmatrix} P_H & R_H \\ -R_H^* & -P_H^T \end{bmatrix} = \begin{bmatrix} \Omega & 0_N \\ 0_N & -\Omega \end{bmatrix},$$

where

$$P_H \equiv T_1^* \omega T_1 + T_2^T \omega^* T_2^* - T_1^* \nu T_2^* - T_2^T \nu^* T_1 = P_H^*, \quad (6'''a)$$

$$R_H \equiv T_1^* \omega T_2 + T_2^T \omega^* T_1^* - T_1^* \nu T_1^* - T_2^T \nu^* T_2 = R_H^T. \quad (6'''b)$$

Let us formulate in another way what we are doing,

$$\begin{aligned} H &= \langle b | H | b \rangle \\ &= \langle b | (T T^{-1}) H (J (T (J J) T^{-1}) J) | b \rangle \\ &= \langle \langle b | T \rangle (T^{-1} H J T J) (J T^{-1} J | b \rangle) \rangle \\ &= \langle B | H_D | B \rangle, \end{aligned}$$

where we have used relation (5') in the last step.

Before going on, a few words about a frequent particular case, namely when  $\nu=0$ . In this (and only this) case the solution is given by  $T_2=0_N$ , and we have to deal with a standard  $N \times N$  diagonalization problem,

$$T_1^* \omega T_1 = \Omega \quad \text{with} \quad T_1^* T_1 = 1_N.$$

Let us now turn back to the general situation. The secular equation of our diagonalization problem is given by

$$\det(HJ - \Omega_j 1_{2N}) \equiv N\text{th degree polynomial in } \Omega_j^2 = 0 \quad \forall j, \quad (7)$$

where the fact that only even powers of  $\Omega_j$  appear, will soon become clear. So our problem will be practically solved if we find a matrix  $T$  which simultaneously diagonalizes the matrix  $HJ$  and satisfies restrictions (5'a), (5'b). The discussion of the existence and uniqueness of such a matrix  $T$  is beyond the scope of this paper. However let us point out a very suggestive fact:

The number of unknown real quantities is *exactly* the same as the number of real relations between them.<sup>21</sup> We have indeed  $(4N^2 + N)$  real unknown quantities:  $2N^2$  for the complex matrix  $T_1$ ,  $2N^2$  for the complex matrix  $T_2$ , and  $N$  for the real diagonal matrix  $\Omega$ . On the other hand, we have  $(4N^2 + N)$  real equations to solve:  $N^2$  for (5''a) (notice that the concerned matrix is Hermitian),  $N(N-1)$  for (5''b) (notice that the concerned matrix is antisymmetric),  $N^2$  for (6''a) (notice that the concerned matrix is Hermitian),  $N(N+1)$  for (6''b) (notice that the concerned matrix is symmetric), and finally  $N$  for (7).

Let us now prove that in the secular equation (7), only even powers of  $\Omega_j$  appear. Relation (6') may be rewritten as follows:

$$HJT = TH_D J$$

or, more explicitly,

$$\begin{bmatrix} \omega & -\nu \\ -\nu^* & -\omega^* \end{bmatrix} \begin{bmatrix} T_1 & T_2 \\ T_2^* & T_1^* \end{bmatrix} = \begin{bmatrix} T_1 & T_2 \\ T_2^* & T_1^* \end{bmatrix} \begin{bmatrix} \Omega & 0_N \\ 0_N & -\Omega \end{bmatrix},$$

in other words, the  $j$ th column of the left half of  $T$  is nothing but the eigenvector associated to the  $j$ th eigenvalue of  $\Omega$  (namely  $\Omega_j$ ), while the  $j$ th column of the right half of  $T$  constitutes the eigenvector associated to  $(-\Omega_j)$ . Then we see that the eigenvectors associated to  $\Omega_j$  and to  $(-\Omega_j)$  are intimately related, and that the secular equation (7) contains only powers of  $\Omega_j^2$ .

Let us assume we found a particular solution<sup>22</sup> (noted  $\bar{T}$ ) of Eq. (6''b). If we now write

$$T \equiv \bar{T}S \quad \text{with } S^{-1} = JS^*J,$$

relation (6'') may be rewritten as follows:

$$S^{-1}(\bar{T}^{-1}HJ\bar{T})S = S^{-1} \begin{bmatrix} Q_H & 0_N \\ 0_N & -Q_H^* \end{bmatrix} S = \begin{bmatrix} \Omega & 0_N \\ 0_N & -\Omega \end{bmatrix},$$

where

$$\begin{aligned} Q_H &\equiv \bar{T}_1^* \omega \bar{T}_1 + \bar{T}_2^* \omega^* \bar{T}_2 \\ &\quad - \bar{T}_1^* \nu \bar{T}_2^* - \bar{T}_2^* \nu^* \bar{T}_1 = Q_H^*. \end{aligned}$$

The solution  $S$  may be written as follows,

$$S = \begin{bmatrix} S_1 & 0_N \\ 0_N & S_1^* \end{bmatrix}, \quad (8)$$

Therefore,

$$S_1^{-1} Q_H S_1 = \Omega$$

with

$$S_1^{-1} = S_1^*.$$

In this way our problem, as in the case  $\nu = 0$ , has been reduced to a standard diagonalization problem of the  $N \times N$  hermitic matrix  $Q_H$ . The matrix  $T$  will be given by

$$T_1 = \bar{T}_1 S_1 \quad \text{and} \quad T_2 = \bar{T}_2 S_1^*.$$

In all usual<sup>23</sup> physical Hamiltonians, we want the  $\{\Omega_j\}$  to be real (and positive) numbers, therefore

$$\det(H) = \prod_{j=1}^N \Omega_j^2 > 0. \quad (9)$$

We can also see that

$$F \equiv (HJ)^2 = \begin{bmatrix} F_1 & F_2 \\ F_2^* & F_1^* \end{bmatrix}$$

where

$$F_1 \equiv \omega^2 - \nu \nu^* = F_1^*,$$

$$F_2 \equiv \nu \omega^* - \omega \nu = -F_2^*.$$

If a matrix  $T$  diagonalizes  $HJ$  necessarily it also diagonalizes  $F$  (the opposite is not true<sup>24</sup>), therefore

$$T^{-1}FT = (H_D J)^2 = \begin{bmatrix} \Omega^2 & 0_N \\ 0_N & \Omega^2 \end{bmatrix}. \quad (10)$$

It follows then that all diagonal elements of  $F_1$  are positive, this is to say

$$\sum_{j=1}^N \{ |\omega_{ij}|^2 - |\nu_{ij}|^2 \} > 0 \quad \forall i. \quad (11)$$

It is clear that conditions (9) and (11) are necessary but in general not sufficient.

The general form (4) for  $T$  leads to

$$T^{-1}FT = \begin{bmatrix} P_F & R_F \\ -R_F^* & P_F^* \end{bmatrix}$$

with

$$P_F \equiv T_1^* F_1 T_1 - T_2^* F_2^* T_2^* + T_1^* F_2 T_2^* - T_2^* F_1^* T_1 = P_F^*,$$

$$R_F \equiv T_1^* F_2 T_1^* - T_2^* F_2^* T_2 + T_1^* F_1 T_2 - T_2^* F_1^* T_1^* = -R_F^*,$$

and relation (10) may be rewritten as follows:

$$P_F = \Omega^2 \quad (10'a)$$

$$R_F = 0_N \quad (10'b)$$

If we assume we found a particular solution<sup>25</sup> (noted  $\bar{T}$ ) of Eq. (10'b), the matrix  $T$  may be written as

$$T = \bar{T}S$$

with  $S$  given by (8) and satisfying

$$S_1^{-1} Q_F S_1 = \Omega^2,$$

$$S_1^{-1} = S_1^*,$$

where

$$Q_F \equiv \bar{T}_1^* F_1 \bar{T}_1 - \bar{T}_2^* F_1^* \bar{T}_2^* + \bar{T}_1^* F_2 \bar{T}_2^* - \bar{T}_2^* F_2^* \bar{T}_1 = Q_F^*.$$

Two immediate corollaries are

$$Q_F = Q_H^2$$

and

$$\det(F) = [\det(Q_F)]^2 = [\det(\Omega)]^4 = \prod_{j=1}^N \Omega_j^4.$$

The preliminary research of  $\bar{T}$  might be of practical importance:  $\bar{T}^{-1}HJ\bar{T}$  might not be diagonal, but it is expected to be much easier to diagonalize than  $HJ$ .

#### 4. PARTICULAR SOLUTION $\bar{T}$

In this section let us discuss a general way to construct a particular solution  $\bar{T}$  of Eq. (10'b). We shall first of all treat the general case  $N=2$ . Let us use the notation





$$H = \langle b | H | b \rangle$$

which defines the  $2N \times 2N$  matrix

$$H = \begin{bmatrix} \omega & \nu \\ \nu^* & \omega^* \end{bmatrix}.$$

The problem will be considered completely solved if we attain the knowledge (as functions of  $\omega$  and  $\nu$ ) of the  $N$  real eigenvalues  $\{\Omega_j\}$  (which define the diagonalized Hamiltonian  $H_D$ ), and of the  $2N \times 2N$  complex matrix  $T$  (which defines the new boson operators  $\langle B | = \langle b | T$  in terms of the old ones). We recall that  $T$  has the form

$$T = \begin{bmatrix} T_1 & T_2 \\ T_2^* & T_1^* \end{bmatrix}$$

which also gives the  $N$  first eigenvalues  $\{\tilde{T}_j\}$  by the  $N \times 2N$  matricial relation

$$\begin{bmatrix} T_1 \\ -\tilde{T}_2^* \end{bmatrix} = [\tilde{T}_1] [\tilde{T}_2] \cdots [\tilde{T}_N],$$

where

$$\tilde{T}_j = \begin{bmatrix} t_j^1 \\ \vdots \\ t_j^N \\ t_j^{N+1} \\ \vdots \\ t_j^{2N} \end{bmatrix}.$$

So the knowledge of  $T$  implies the knowledge of  $4N^2$  real numbers (only  $2N^2$  if  $T$  is real). We recall that

$$J = \begin{bmatrix} 1_N & 0_N \\ 0_N & -1_N \end{bmatrix}.$$

Method I:

(1) Find the roots of the secular equation

$$\det(HJ - \lambda 1_{2N}) = N\text{th degree polynomial in } \lambda^2 = 0.$$

Then  $\Omega_j = |\lambda_j|$  ( $j = 1, 2, \dots, N$ ).

(2) Write, for each value of  $j$ , the set of  $4N$  real equations (only  $2N$  if  $T$  is real)

$$[(HJ - \Omega_j 1_{2N}) \tilde{T}_j]_k = 0 \quad (k = 1, 2, \dots, 2N),$$

where by  $[\dots]_k$  we are noting the  $k$ th component of the vector. Then eliminate an arbitrary one between them and replace it by the real one

$$\sum_{k=1}^N |t_j^k|^2 - \sum_{k=N+1}^{2N} |t_j^k|^2 = 1. \quad (17)$$

We have in this way a set of  $4N$  independent real equations (only  $2N$  if  $T$  is real) which in principle leads to

the knowledge of the  $2N$  complex numbers  $\{t_j^k\}$  associated to the chosen value of  $j$ . An example of how to use this method is given in Appendix A.

(2') Alternative possibility for step (2): Find a particular solution  $\bar{T}$  of the equations

$$(\bar{T}_1^* \omega \bar{T}_2 + \bar{T}_2^* \omega^* \bar{T}_1^* - \bar{T}_1^* \nu \bar{T}_1^* - \bar{T}_2^* \nu^* \bar{T}_2)_{ij} = 0 \quad (i \geq j),$$

where by  $(\dots)_{ij}$  we note the  $ij$ th element of the matrix, and where the norm relation (17) must also be satisfied.

(3') Calculate the matrix

$$Q_H = \bar{T}_1^* \omega \bar{T}_1 + \bar{T}_2^* \omega^* \bar{T}_2^* - \bar{T}_1^* \nu \bar{T}_2^* - \bar{T}_2^* \nu^* \bar{T}_1$$

and solve the standard diagonalization problem

$$(S_1^{-1} Q_H S_1)_{ij} = \Omega_j \delta_{ij}$$

with  $S_1^{-1} = S_1^*$  and  $\delta_{ij} = \text{Kroenecker's delta}$ .

(4')  $T$  is given by

$$T_1 = \bar{T}_1 S_1 \quad \text{and} \quad T_2 = \bar{T}_2 S_1^*.$$

Method II:

(1) The same as step (1) of Method I.

(2) Calculate the matrix

$$F_1 = \begin{bmatrix} f_{11} & \dots & f_{1N} \\ \vdots & & \vdots \\ f_{N1}^* & \dots & f_{NN} \end{bmatrix} = \omega^2 - \nu \nu^*,$$

$$F_2 = \begin{bmatrix} 0 & \tilde{f}_{12} \exp(i\varphi_{12}) & \dots & \tilde{f}_{1N} \exp(i\varphi_{1N}) \\ -\tilde{f}_{12} \exp(i\varphi_{12}) & 0 & \dots & \tilde{f}_{2N} \exp(i\varphi_{2N}) \\ \vdots & \vdots & \ddots & \vdots \\ -\tilde{f}_{1N} \exp(i\varphi_{1N}) & -\tilde{f}_{2N} \exp(i\varphi_{2N}) & \dots & 0 \end{bmatrix}$$

$$= \nu \omega^* - \omega \nu.$$

(3) Write, for each one of the  $\frac{1}{2}N(N-1)$  values of  $(ij)$  [ $ij = 12, 13, \dots, 1N, 23, 24, \dots, 2N, \dots, (N-1)N$ ], the  $2N \times 2N$  matrix

$$\bar{T}^{ij} = \begin{bmatrix} \bar{T}_1^{ij} & \bar{T}_2^{ij} \\ (\bar{T}_2^{ij})^* & (\bar{T}_1^{ij})^* \end{bmatrix},$$

where

$\bar{T}_1^{ij}$  is given by expression (13),

and

$\bar{T}_2^{ij}$  is given:

by expressions (14) and (14a) if  $f_{ii} \neq f_{jj}$ ;

by expressions (14) and (14b) if  $f_{ii} = f_{jj}$  and  $\Re(f_{ij}) \neq 0$ ;

by expressions (14) and (14c) if  $f_{ii} = f_{jj}$  and  $\Re(f_{ij}) = 0$ .

(4) Calculate the  $2N \times 2N$  matrix

$$\bar{T} = \bar{T}^{12} \bar{T}^{13} \dots \bar{T}^{1N} \bar{T}^{23} \bar{T}^{24} \dots \bar{T}^{2N} \dots \bar{T}^{N-1,N}$$

which will now be expressed in terms of the  $N(N-1)$  real numbers  $\{\psi_{ij}\}$  and  $\{\chi_{ij}\}$ . Then present  $\bar{T}$  in the form

$$\bar{T} \equiv \begin{bmatrix} \bar{T}_1 & \bar{T}_2 \\ \bar{T}_2^* & \bar{T}_1^* \end{bmatrix}$$

which leads to the knowledge of  $\bar{T}_1$  and  $\bar{T}_2$  separately.

(5) Determine  $\{\psi_{ij}\}$  and  $\{\chi_{ij}\}$  by solving the  $N(N-1)$  real equations given by the matricial relation

$$\bar{T}_1^* F_2 \bar{T}_1^* - \bar{T}_2^* F_2^* \bar{T}_2 + \bar{T}_1^* F_1 \bar{T}_2 - \bar{T}_2^* F_1^* \bar{T}_1^* = 0_N.$$

Substitute the solutions in the expression of  $\bar{T}$  obtained in step (4), which will now be a function of  $\{f_{ij}\}$ ,  $\{\bar{f}_{ij}\}$ , and  $\{\varphi_{ij}\}$ .

(6) Calculate the  $N \times N$  matrix

$$Q_F = \bar{T}_1^* F_1 \bar{T}_1 - \bar{T}_2^* F_1^* \bar{T}_2 + \bar{T}_1^* F_2 \bar{T}_2 - \bar{T}_2^* F_2^* \bar{T}_1.$$

(7) Proceed to a standard diagonalization of the hermitic matrix  $Q_F$  by a unitary matrix  $S_1$  presented in the following form:

$$S_1 \equiv (\tilde{S}_1)(\tilde{S}_2) \cdots (\tilde{S}_N).$$

To perform this, write, for each value of  $j$ , the set of  $2N$  real equations

$$[(Q_F - \Omega_j^2 1_N) \tilde{S}_j]_k = 0 \quad (k=1, 2, \dots, N).$$

Then eliminate an arbitrary one between them and replace it by the real equation

$$\|\tilde{S}_j\| = 1.$$

The solution of this set of  $2N$  real equations (only  $N$  if  $S_1$  is real) gives the vector  $\tilde{S}_j$ .

(8) Calculate the matrix

$$T'_1 = \bar{T}_1 S_1 \quad \text{and} \quad T'_2 = \bar{T}_2 S_1^*$$

and then

$$T' = \begin{bmatrix} T'_1 & T'_2 \\ (T'_2)^* & (T'_1)^* \end{bmatrix}.$$

(9) Calculate the matrix

$$H' = (T')^{-1} H J T' J$$

and enter in step (2) or step (2') of Method I.

An example of use of this method is given in Appendix B.

*Method III:* This method is applicable only for the research of the eigenvalues  $\{\Omega_j\}$  and only for some particular cases:

$$1st \text{ case: } \omega + \omega^* = \pm(\nu + \nu^*)$$

Find the roots of the secular equations

$$\det[(\omega - \omega^* + \nu - \nu^*)^2 - \mu 1_N] = 0,$$

then

$$\Omega_j = \frac{1}{2} \sqrt{\mu_j} \quad (j=1, 2, \dots, N).$$

$$2nd \text{ case: } \omega + \omega^* = \pm i(\nu - \nu^*)$$

Find the roots of the secular equation

$$\det[(\omega - \omega^*) - i(\nu + \nu^*)]^2 - \mu 1_N = 0,$$

then

$$\Omega_j = \frac{1}{2} \sqrt{\mu_j} \quad (j=1, 2, \dots, N).$$

$$3rd \text{ case: } \omega - \omega^* = \nu - \nu^* = 0_N$$

Find the roots of the equation

$$\sum_{n=0}^N (-1)^n C_n \mu^{N-n} = 0,$$

where  $C_n$  is given in Appendix D with

$$A \equiv -\omega + \nu \quad \text{and} \quad B \equiv -\omega - \nu$$

and then

$$\Omega_j = \sqrt{\mu_j} \quad (j=1, 2, \dots, N).$$

$$4th \text{ case: } \omega - \omega^* = \nu + \nu^* = 0_N$$

Find the roots of the equation

$$\sum_{n=0}^N (-1)^n C_n \mu^{N-n} = 0,$$

where  $C_n$  is given in Appendix D with

$$A \equiv \nu - i\omega \quad \text{and} \quad B \equiv \nu + i\omega$$

and then

$$\Omega_j = \sqrt{\mu_j} \quad (j=1, 2, \dots, N).$$

Examples of the use of this method are given in Appendix C.

## 7. CONCLUSION

Let us conclude by saying that the exposed method for diagonalizing any Hamiltonian of  $N$  bilinearly interacting bosons is absolutely equivalent to the so-called "equation-of-motion approach." However systematic exploitation of the peculiar boson properties had led to a concise mathematical formulation which allows for the establishment of operational rules. We have only spoken of  $N$  bosons; nevertheless the method is equally applicable to  $N$  families (or branches) of bosons, by simple identification of the boson operators ( $b_1 \equiv b_q$ ,  $b_2 \equiv b_{-q}$ , etc.) as it was done, for example, in Refs. 1, 16, 17, and 18.

Finally let us compare the different methods presented in this paper. Method I [steps (1) and (2)] should be considered the most standard way of performing the diagonalization, however if the matrix  $H$  is rather complicated (low symmetry, no zeros), the more delayed procedure indicated in Method I [steps (1), (2'), (3'), and (4')] could be preferable. Furthermore, if  $H$  is very complicated, the highly delayed procedure indicated in Method II could be worth while. If we are interested only in the eigenvalues (as it is frequently the case in statistical mechanics), there is no doubt that Method III should be adopted if we are faced with one of its four cases; if not, the problem will be solved by Method I [step (1)].

## ACKNOWLEDGMENTS

We acknowledge with pleasure early and fruitful criticism from J. Tavernier as well as useful discussions with R. Tabensky, J.W. Furtado Valle, R. Feijóo, and R. Lobo.



## APPENDIX A

Let us treat, by Method I, the cases  $N=1$  and  $N=2$ . For  $N=1$  we have  $\omega \in \mathbb{R}$  and  $\nu = |\nu| \exp(i\varphi) \in \mathbb{C}$ . The secular equation is

$$\begin{vmatrix} \omega - \lambda & -|\nu| \exp(i\varphi) \\ |\nu| \exp(-i\varphi) & -\omega - \lambda \end{vmatrix} = 0$$

hence  $\lambda = \pm(\omega^2 - |\nu|^2)^{1/2}$  hence  $\Omega = (\omega^2 - |\nu|^2)^{1/2}$ . We see that it must be  $\omega > |\nu|$ . Let us propose

$$\bar{T}_1 = \cosh \psi \quad \text{and} \quad \bar{T}_2 = \exp(i\chi) \sinh \psi.$$

Therefore [performing step (2') of Method I],

$$\chi = \varphi \quad \text{and} \quad \tanh 2\psi = |\nu|/\omega,$$

hence

$$\bar{T}_1 = \frac{1}{\sqrt{2}} \frac{[\omega + (\omega^2 - |\nu|^2)^{1/2}]^{1/2}}{(\omega^2 - |\nu|^2)^{1/4}}$$

and

$$\bar{T}_2 = \frac{\exp(i\varphi)}{\sqrt{2}} \frac{[\omega - (\omega^2 - |\nu|^2)^{1/2}]^{1/2}}{(\omega^2 - |\nu|^2)^{1/4}}.$$

We may then verify that  $Q_H = (\omega^2 - |\nu|^2)^{1/2}$ , as it is natural. In this case, obviously  $T = \bar{T}$ .

For  $N=2$  we shall only find the eigenvalues. The most general situation is given by

$$\omega \equiv \begin{bmatrix} \omega_{11} & \omega_{12} \\ \omega_{12}^* & \omega_{22} \end{bmatrix} \quad \text{and} \quad \nu \equiv \begin{bmatrix} \nu_{11} & \nu_{12} \\ \nu_{12} & \nu_{22} \end{bmatrix}$$

with  $\omega_{11}, \omega_{22}$  being real numbers and the rest being complex. The secular equation is given by

$$\begin{vmatrix} \omega_{11} - \lambda & \omega_{12} & -\nu_{11} & -\nu_{12} \\ \omega_{12}^* & \omega_{22} - \lambda & -\nu_{12} & -\nu_{22} \\ \nu_{11}^* & \nu_{12}^* & -\omega_{11} - \lambda & -\omega_{12}^* \\ \nu_{12}^* & \nu_{22}^* & -\omega_{12} & -\omega_{22} - \lambda \end{vmatrix} = \lambda^4 - C_1 \lambda^2 + C_2 = 0,$$

where

$$C_1 \equiv \omega_{11}^2 + \omega_{22}^2 + 2|\omega_{12}|^2 - |\nu_{11}|^2 - |\nu_{22}|^2 - 2|\nu_{12}|^2$$

and

$$\begin{aligned} C_2 \equiv & \omega_{11}^2 \omega_{22}^2 + |\omega_{12}|^4 - 2\omega_{11}\omega_{22}|\omega_{12}|^2 - \omega_{11}^2|\nu_{22}|^2 - \omega_{22}^2|\nu_{11}|^2 \\ & - 2(\omega_{11}\omega_{22} + |\omega_{12}|^2)|\nu_{12}|^2 + |\nu_{11}|^2|\nu_{22}|^2 + |\nu_{12}|^4 \\ & - 2\mathcal{R}(\omega_{12}^* \nu_{11}^* \nu_{22}) - 2\mathcal{R}(\nu_{11} \nu_{22} \nu_{12}^*) \\ & + 4\omega_{11}\mathcal{R}(\omega_{12} \nu_{12}^* \nu_{22}) + 4\omega_{22}\mathcal{R}(\omega_{12} \nu_{12} \nu_{11}^*). \end{aligned}$$

Therefore,

$$\Omega_{1,2} = \pm \left[ \frac{C_1}{2} \pm \left( \frac{C_1^2}{4} - C_2 \right)^{1/2} \right]^{1/2}.$$

We see that it must be

$$C_1 \geq 0 \quad \text{and} \quad C_1^2 \geq 4C_2 \geq 0.$$

The particular case  $\nu_{11} = \nu_{22} = 0$  and  $\omega_{12} = \nu_{12} \in \mathbb{R}$  appears in Ref. 18. On the other hand, if we assume that  $\omega_{22} = \omega_{12} = \nu_{22} = \nu_{12} = 0$ , we reobtain the case  $N=1$ .

## APPENDIX B

We shall treat here the case  $N=2$  in the particular case  $\omega_{11} = \omega_{22} = 1$ ,  $\nu_{11} = \nu_{22} = 0$ , and  $\omega_{12} = \nu_{12} \in \mathbb{R}$ . The eigenvalues have already been obtained in Appendix A:

$$\Omega_{1,2} = \sqrt{1 \pm 2\omega_{12}}.$$

Therefore, it must be  $|\omega_{12}| < \frac{1}{2}$ . We verify immediately that  $F_2 = 0_2$ , hence  $\bar{T} = \mathbf{1}_4$ , therefore

$$Q_F = F_1 = \begin{bmatrix} 1 & 2\omega_{12} \\ 2\omega_{12} & 1 \end{bmatrix} \quad \text{and} \quad H' = H.$$

Now we enter into step (2) of Method I. The equations to determine  $T$  are

$$[(HJ - \sqrt{1 + 2\omega_{12}} \mathbf{1}_4) \bar{T}_1]_k = 0 \quad (k=1, 2, 3),$$

$$(t_1^1)^2 + (t_1^2)^2 - (t_1^3)^2 - (t_1^4)^2 = 1,$$

$$[(HJ - \sqrt{1 - 2\omega_{12}} \mathbf{1}_4) \bar{T}_2]_{k=0} = 0 \quad (k=1, 2, 3),$$

$$(t_2^1)^2 + (t_2^2)^2 - (t_2^3)^2 - (t_2^4)^2 = 1.$$

The solution (attained through very boring calculations!) is given by

$$T_1 = \begin{bmatrix} t_1^1 & t_1^2 \\ t_1^3 & -t_1^4 \end{bmatrix} \quad \text{and} \quad T_2 = \begin{bmatrix} t_2^1 & t_2^2 \\ t_2^3 & -t_2^4 \end{bmatrix}$$

with

$$t_1^1 = \frac{|\omega_{12}|}{D_1}, \quad t_1^3 = \frac{\omega_{12}}{|\omega_{12}|} \frac{1 + \omega_{12} - \sqrt{1 + 2\omega_{12}}}{D_1},$$

$$t_2^1 = \frac{|\omega_{12}|}{D_2}, \quad t_2^3 = \frac{\omega_{12}}{|\omega_{12}|} \frac{-1 + \omega_{12} + \sqrt{1 - 2\omega_{12}}}{D_2},$$

$$D_1 \equiv \sqrt{2} [\omega_{12}^2 - (1 + \omega_{12} - \sqrt{1 + 2\omega_{12}})^2]^{1/2},$$

$$D_2 \equiv \sqrt{2} [\omega_{12}^2 - (1 - \omega_{12} - \sqrt{1 - 2\omega_{12}})^2]^{1/2}.$$

## APPENDIX C

We shall treat here, by Method III, the case  $N=3$  for  $\omega$  and  $\nu$  a real matrix. The secular equation can be written as follows

$$\mu^3 - C_1 \mu^2 + C_2 \mu - C_3 = 0,$$

where

$$C_1 = \omega_{11}^2 + \omega_{22}^2 + \omega_{33}^2 - \nu_{11}^2 - \nu_{22}^2 - \nu_{33}^2$$

$$+ 2(\omega_{12}^2 + \omega_{13}^2 + \omega_{23}^2 - \nu_{12}^2 - \nu_{13}^2 - \nu_{23}^2),$$

$$C_2 =$$

$$\begin{aligned} & (\omega_{11}\omega_{22} + \nu_{11}\nu_{22} - \omega_{12}^2 - \nu_{12}^2)^2 - (\omega_{11}\nu_{22} + \omega_{22}\nu_{11} - 2\omega_{12}\nu_{12})^2 \\ & + (\omega_{22}\omega_{33} + \nu_{22}\nu_{33} - \omega_{23}^2 - \nu_{23}^2)^2 - (\omega_{22}\nu_{33} + \omega_{33}\nu_{22} - 2\omega_{23}\nu_{23})^2 \\ & + (\omega_{11}\omega_{33} + \nu_{11}\nu_{33} - \omega_{13}^2 - \nu_{13}^2)^2 - (\omega_{11}\nu_{33} + \omega_{33}\nu_{11} - 2\omega_{13}\nu_{13})^2 \\ & + 2[(\omega_{11}\omega_{23} + \nu_{11}\nu_{23} - \omega_{12}\omega_{13} - \nu_{12}\nu_{13})^2 \\ & - (\omega_{11}\nu_{23} + \nu_{11}\omega_{23} - \omega_{12}\nu_{13} - \omega_{13}\nu_{12})^2 \\ & + (\omega_{22}\omega_{13} + \nu_{22}\nu_{13} - \omega_{12}\omega_{23} - \nu_{12}\nu_{23})^2 \\ & - (\omega_{22}\nu_{13} + \nu_{22}\omega_{13} - \omega_{12}\nu_{23} - \omega_{23}\nu_{12})^2 \\ & + (\omega_{33}\omega_{12} + \nu_{33}\nu_{12} - \omega_{13}\omega_{23} - \nu_{13}\nu_{23})^2 \\ & - (\omega_{33}\nu_{12} + \nu_{33}\omega_{12} - \omega_{13}\nu_{23} - \omega_{23}\nu_{13})^2], \end{aligned}$$

$$C_3 = \begin{vmatrix} \omega_{11} - \nu_{11} & \omega_{12} - \nu_{12} & \omega_{13} - \nu_{13} \\ \omega_{12} - \nu_{12} & \omega_{22} - \nu_{22} & \omega_{23} - \nu_{23} \\ \omega_{13} - \nu_{13} & \omega_{23} - \nu_{23} & \omega_{33} - \nu_{33} \end{vmatrix} \\ \times \begin{vmatrix} \omega_{11} + \nu_{11} & \omega_{12} + \nu_{12} & \omega_{13} + \nu_{13} \\ \omega_{12} + \nu_{12} & \omega_{22} + \nu_{22} & \omega_{23} + \nu_{23} \\ \omega_{13} + \nu_{13} & \omega_{23} + \nu_{23} & \omega_{33} + \nu_{33} \end{vmatrix}.$$

The eigenvalues are given by

$$\Omega_j = +\sqrt{\mu_j} \quad (j=1, 2, 3).$$

If in the present secular equation we take the particular case  $\omega_{33} = \nu_{33} = \omega_{13} = \omega_{23} = \nu_{12} = \nu_{23} = 0$ , we easily verify the consistence with the secular equation obtained in Appendix A for  $N=2$ .

## APPENDIX D

We want to calculate the determinant

$$\Delta \equiv \begin{vmatrix} \lambda 1_N & A \\ B & \lambda 1_N \end{vmatrix},$$

where

$$A \equiv \begin{bmatrix} a_{11} & \dots & a_{1N} \\ \vdots & & \vdots \\ a_{1N} & \dots & a_{NN} \end{bmatrix} = A^T, \\ B \equiv \begin{bmatrix} b_{11} & \dots & b_{1N} \\ \vdots & & \vdots \\ b_{1N} & \dots & b_{NN} \end{bmatrix} = B^T$$

with  $\{a_{ij}\}$  and  $\{b_{ij}\}$  being complex numbers. A long, but not complicated, inductive process leads to

$$\Delta = \sum_{n=0}^N (-1)^n C_n \lambda^{2(N-n)},$$

where

$$C_0 = 1$$

$$C_1 = \sum_{i=1}^N \partial_{ii} b_{ii} + 2 \sum_{i < j} \partial_{ij} b_{ij},$$

$$C_n = \sum_{\{\text{all minors}\}} (\alpha^{(n)} \beta^{(n)}) \left( \left[ \frac{N!}{n!(N-n)!} \right]^2 \text{terms} \right),$$

$$C_N = |A| |B|,$$

$\alpha^{(n)} \equiv$  determinant of an  $n \times n$  minor of matrix  $A$ , constructed without touching the positions of the elements  $a_{ij}$ .

$\beta^{(n)} \equiv$  determinant of an  $n \times n$  minor of matrix  $B$ , which is obtained by making  $a_{ij} \rightarrow b_{ij}$  in  $\alpha^{(n)}$ .

In order to clarify the use of this method, we present here the results for  $N=2$  and  $N=3$ ;

$$\begin{vmatrix} \lambda & 0 & a_{11} & a_{12} \\ 0 & \lambda & a_{12} & a_{22} \\ b_{11} & b_{12} & \lambda & 0 \\ b_{12} & b_{22} & 0 & \lambda \end{vmatrix} \\ = \lambda^4 - (a_{11}b_{11} + a_{22}b_{22} + 2a_{12}b_{12})\lambda^2 + \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} \begin{vmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{vmatrix},$$

$$\begin{vmatrix} \lambda & 0 & 0 & a_{11} & a_{12} & a_{13} \\ 0 & \lambda & 0 & a_{12} & a_{22} & a_{23} \\ 0 & 0 & \lambda & a_{13} & a_{23} & a_{33} \\ b_{11} & b_{12} & b_{13} & \lambda & 0 & 0 \\ b_{12} & b_{22} & b_{23} & 0 & \lambda & 0 \\ b_{13} & b_{23} & b_{33} & 0 & 0 & \lambda \end{vmatrix} \\ = \lambda^6 - \lambda^4 (a_{11}b_{11} + a_{22}b_{22} + a_{33}b_{33} + 2a_{12}b_{12} + 2a_{13}b_{13} + 2a_{23}b_{23}) \\ + \lambda^2 \left\{ \begin{vmatrix} a_{22} & a_{23} \\ a_{23} & a_{33} \end{vmatrix} \begin{vmatrix} b_{22} & b_{23} \\ b_{23} & b_{33} \end{vmatrix} + \begin{vmatrix} a_{11} & a_{13} \\ a_{13} & a_{33} \end{vmatrix} \begin{vmatrix} b_{11} & b_{13} \\ b_{13} & b_{33} \end{vmatrix} \right. \\ \left. + \begin{vmatrix} a_{11} & a_{12} \\ a_{12} & a_{22} \end{vmatrix} \begin{vmatrix} b_{11} & b_{12} \\ b_{12} & b_{22} \end{vmatrix} \right. \\ \left. + 2 \begin{vmatrix} a_{12} & a_{23} \\ a_{13} & a_{33} \end{vmatrix} \begin{vmatrix} b_{12} & b_{23} \\ b_{13} & b_{33} \end{vmatrix} \right. \\ \left. + 2 \begin{vmatrix} a_{12} & a_{22} \\ a_{13} & a_{23} \end{vmatrix} \begin{vmatrix} b_{12} & b_{22} \\ b_{13} & b_{23} \end{vmatrix} + 2 \begin{vmatrix} a_{11} & a_{12} \\ a_{13} & a_{23} \end{vmatrix} \begin{vmatrix} b_{11} & b_{12} \\ b_{13} & b_{23} \end{vmatrix} \right\} \\ - \begin{vmatrix} a_{11} & a_{12} & a_{13} \\ a_{12} & a_{22} & a_{23} \\ a_{13} & a_{23} & a_{33} \end{vmatrix} \begin{vmatrix} b_{11} & b_{12} & b_{13} \\ b_{12} & b_{22} & b_{23} \\ b_{13} & b_{23} & b_{33} \end{vmatrix}.$$

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<sup>19</sup>Eventual terms linear in boson operators can be easily removed by defining new boson operators related to the old ones by  $a = b + \mu$  and  $a^* = b^* + \mu^*$ , where  $\mu \in \mathbb{C}$ . Additive constants in Hamiltonians are not going to be explicitly written in this paper, because of their simpleness and quite frequent irrelevance.

<sup>20</sup>In any case  $\mathcal{H}$  is going to conserve the number of  $B$  bosons, which are to be introduced.

<sup>21</sup>This is not a *sufficient* condition for the existence of the solution; therefore strictly speaking it guarantees nothing beyond

a strong suspicion.

<sup>22</sup>Equation (6'''b) of course admits a great number of solutions, from which only one (independent) simultaneously satisfies (6'''a).

<sup>23</sup>Hamiltonians adapted to describe displacive phase transitions might constitute an exception.

<sup>24</sup>The reason is that the eigenvalues  $|\Omega_j|$  and  $-|\Omega_j|$  lead, in  $F$ , to a degenerate bidimensional subspace related to the eigenvalue  $\Omega_j^2$ . It is clear that  $\nu \neq 0_N$  and  $\nu\omega^* - \omega\nu = 0_N$  are compatible (an example is given in Appendix B).

<sup>25</sup>Every  $\bar{T}$  is also a  $\bar{\bar{T}}$ , but the opposite is not true.

<sup>26</sup>If  $f_{11} = f_{22}$  and  $f_{12} = 0$  the secular equation for  $F$  leads to the roots  $\Omega_{1,2}^2 = f_{11} \pm i\tilde{f}_{12}$ .