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On the diagonalization of the general quadratic Hamiltonian for coupled harmonic oscillators

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It is shown that the general quadratic Hamiltonian for coupled harmonic oscillators can be diagonalized, provided the matrix of the quadratic form is positive definite. This condition is also necessary if the frequencies of the resulting uncoupled oscillators are to be positive. The construction of a diagonalizing matrix follows the usual procedure as in the Hermitian case; the only difference being a change of the metric from

$I = \begin{pmatrix}1 & \\ & 1\end{pmatrix}$ to $J = \begin{pmatrix}1 & \\ & -1\end{pmatrix}$.

1. INTRODUCTION

It is well known that the eigenvalues for a system of n coupled harmonic oscillators can be found by means of a principal axis transformation. Thus, given the Hamiltonian

$$H = (a^\dagger a) H \binom{a}{a^\dagger}, \tag{1}$$

with $(a^\dagger a) = (a_1^\dagger \cdots a_n^\dagger, a_1 \ldots a_n)$ and $H = \begin{pmatrix}\alpha & \beta \\ \beta* & \alpha*\end{pmatrix} = H^\dagger$, a $2n$ by $2n$ regular matrix A is sought such that

$$(A^{-1})^\dagger H (A^{-1}) = H' \tag{2}$$

is diagonal. [Notation: Hermitian conjugation of matrices and operators is denoted by a dagger. Thus $\binom{a}{a^\dagger}^\dagger = (a^\dagger a)$. A star denotes complex conjugation and a tilde stands for the transpose.] Once A has been found, the eigenvalues can be read from the uncoupled form

$$H = (b^\dagger b) H' \binom{b}{b^\dagger} = \sum \hbar\omega_i b_i^\dagger b_i + \text{const}, \tag{3}$$

where

$$\binom{b}{b^\dagger} = A \binom{a}{a^\dagger} \tag{4}$$

are the new boson operators. In order for the b's to satisfy the boson commutation rules, A must fulfill[1,2]

$$A = \begin{pmatrix}\lambda & \mu \\ \mu* & \lambda*\end{pmatrix}, \tag{5a}$$

and

$$AJA^\dagger = J, \tag{5b}$$

where $J = \begin{pmatrix}1 & \\ & -1\end{pmatrix}$. The question now arises: What conditions on the Hamiltonian matrix H are sufficient to ensure the existence of a matrix A satisfying (2) and (5), and how is one going to construct A? It seems that such conditions have not been spelled out in the literature, though a set of operational rules to facilitate the computation of A (when it exists), has recently been formulated.[1] Reference 1 also contains a fairly broad list of interesting applications to physical problems.

The purpose of this note is to show that A exists and can be calculated by following routine diagonalization procedures, provided H is positive definite, that is,

$$(x)^\dagger H (x) > 0, \quad \forall (x) \neq (0). \tag{6}$$

Equivalently, since H is Hermitian, the eigenvalues of H should be positive. [Note that, in general, the eigenvalues of H are not the diagonal elements of H' in Eq. (2).] As we shall presently show, Condition (6) is also necessary, if the frequencies of the uncoupled Hamiltonian (3) are to be positive. Indeed, let $H' = \begin{pmatrix}\gamma & \\ & \gamma'\end{pmatrix}$. Since H is Hermitian, γ and γ' are real diagonal n by n matrices with diagonal elements γ_i and γ_i'. Let $A = \begin{pmatrix}\lambda & \mu \\ \mu* & \lambda*\end{pmatrix}$. Then, by Eq. (5),

$$A^{-1} = JA^\dagger J = \begin{pmatrix}\lambda^\dagger & -\tilde{\mu} \\ -\mu^\dagger & \tilde{\lambda}\end{pmatrix}.$$

Equation (2), therefore, reads

$$\begin{pmatrix}\lambda & -\mu \\ -\mu* & \lambda*\end{pmatrix}\begin{pmatrix}\alpha & \beta \\ \beta* & \alpha*\end{pmatrix}\begin{pmatrix}\lambda^\dagger & -\tilde{\mu} \\ -\mu^\dagger & \tilde{\lambda}\end{pmatrix} = \begin{pmatrix}\gamma & \\ & \gamma'\end{pmatrix}. \tag{7}$$

Performing the matrix multiplication, we find $\gamma = \gamma'$, that is, $H' = \begin{pmatrix}\gamma & \\ & \gamma\end{pmatrix}$. Thus, the uncoupled Hamiltonian (3) is explicitly given by

$$H = \sum_{i=1}^{n} 2\gamma_i (b_i^\dagger b_i + \tfrac{1}{2}). \tag{8}$$

Accordingly, if the frequencies $\omega_i = 2\gamma_i/\hbar$ are to be positive, the Hamiltonian matrix

$$H = A^\dagger H' A = (H'^{1/2}A)^\dagger (H'^{1/2}A) \tag{9}$$

must be positive definite.

Before turning to the discussion of diagonalization, let us recast Eq. (2), with the aid of (5), into the usual eigenvalue form, namely,

$$(HJ)A^\dagger = A^\dagger (H'J). \tag{10}$$

Note that HJ is, in general, not Hermitian. Another useful form is

$$AJHJA^\dagger = H'. \tag{11}$$

In Sec. 2 we shall first establish the existence of a diagonalizing matrix A, and then show how to actually construct it. As it turns out, the construction follows exactly the same procedure as in the Hermitian case, the only difference being the change of the metric from $I = \begin{pmatrix}1 & \\ & 1\end{pmatrix}$ to $J = \begin{pmatrix}1 & \\ & -1\end{pmatrix}$. Finally, in the Appendix, we amend a shortcoming in Ref. 2, wherein a related problem is discussed, namely, given the diagonalizing matrix A, find the transformation brackets connecting base states of the old operators $(a_i, a_i^\dagger)$ with those of the new operators $(b_i, b_i^\dagger)$.

2. DIAGONALIZATION

A. Existence

Let H be a positive definite $2n$ by $2n$ Hermitian

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matrix. Since JHJ shares the same properties, there exists a unitary matrix U such that

$$U^\dagger JHJU = E \tag{12}$$

is a diagonal positive matrix. Define

$$V = UE^{-1/2}, \tag{13}$$

Then V is regular and satisfies

$$V^\dagger JHJV = 1. \tag{14}$$

Let P be a unitary matrix diagonalizing the Hermitian matrix $V^\dagger JV$, that is,

$$P^\dagger V^\dagger JVP = \eta, \qquad \eta_{ij} = \delta_{ij}\eta_i. \tag{15}$$

Then

$$W = VP \tag{16}$$

satisfies

$$W^\dagger JW = \eta, \tag{17}$$

and

$$W^\dagger JHJW = 1. \tag{18}$$

Equation (17) is a congruence transformation on the matrix J conserving the number of positive and negative elements in J (Sylvester's law of inertia[3]). Hence, n of the η_i's are positive and n are negative. Let θ be a diagonal matrix with elements

$$\theta_{ij} = \delta_{ij}|\eta_i|. \tag{19}$$

Then

$$\zeta = ((\zeta_1)(\zeta_2)\cdots(\zeta_{2n})) \equiv W\theta^{-1/2} \tag{20}$$

satisfies

$$(\zeta_i)^\dagger J(\zeta_j) = \delta_{ij}\eta_i/|\eta_i|, \tag{21}$$

and

$$(\zeta_i)^\dagger JHJ(\zeta_j) = \delta_{ij}|\eta_i|^{-1}. \tag{22}$$

Now rearrange the column vectors (ζ_i) into a new matrix

$$Z = ((z_1\cdots(z_n)(\hat{z}_1)\cdots(\hat{z}_n)) \tag{23}$$

such that the vectors (z_i) have positive norm, namely,

$$(z_i)^\dagger J(z_j) = \delta_{ij}, \qquad i,j = 1, \ldots, n, \tag{24a}$$

and the vectors $(\hat{z}_i)$ have negative norm

$$(\hat{z}_i)^\dagger J(\hat{z}_j) = -\delta_{ij}, \qquad i,j = 1, \ldots, n. \tag{24b}$$

Since Z satisfies

$$Z^\dagger JZ = J, \tag{25}$$

and

$$Z^\dagger JHJZ = H', \tag{26}$$

we see that $A = Z^\dagger$ is a solution to the diagonalization problem [Eqs. (5) and (11)]. We note, in passing, that the same proof applies to more general metrics: the diagonal matrix J could have any number $0 \leqslant k \leqslant 2n$ of positive elements and, correspondingly, $2n-k$ negative elements. Equation (26), with the aid of Eq. (25), can be rewritten in the form

$$(HJ)Z = Z(JH') = Z\begin{pmatrix}\gamma & \\ & -\gamma\end{pmatrix}. \tag{27}$$

Thus, (z_i) are eigenvectors of HJ with eigenvalues γ_i, and similarily, $(\hat{z}_i)$ are eigenvectors of HJ with eigenvalues $-\gamma_i$.

B. Construction

The actual construction of a diagonalizing matrix $Z = A^\dagger$ follows closely the procedure employed in the Hermitian case, the only difference being the change of the metric from $I = \begin{pmatrix}1 & \\ & 1\end{pmatrix}$ to $J = \begin{pmatrix}1 & \\ & -1\end{pmatrix}$. We shall make use of the following observations:

(a) The eigenvectors of J have nonvanishing norm. Let

$$HJ(x_i) = \gamma_i(x_i). \tag{28}$$

Since H is positive definite and J is regular,

$$(x_i)^\dagger JHJ(x_i) = \gamma_i(x)^\dagger J(x_i) > 0. \tag{29}$$

Thus $(x_i)^\dagger J(x_i) \gtrless 0$ according to $\gamma_i \gtrless 0$, and (x_i) can be normalized to satisfy

$$(x_i)^\dagger J(x_i) = \pm 1, \qquad \gamma_i \gtrless 0. \tag{30}$$

(b) Eigenvectors belonging to different eigenvalues are orthogonal with respect to J. Indeed, if

$$HJ(x_i) = \gamma_i(x_i) \quad \text{and} \quad H\,J(x_j) = \gamma_j(x_k), \tag{31}$$

then

$$(x_j)^\dagger JHJ(x_i) = \gamma_i(x_j)^\dagger J(x_i) = \gamma_j(x_j)^\dagger J(x_i). \tag{32}$$

(c) If γ_i is a multiple root of $\det(HJ - \gamma I)$ with multiplicity k, there exist exactly k linearly independent eigenvectors having γ_i as their common eigenvalue. Indeed, let Z satisfy Eqs. (25) and (26). Since the ranks of the two matrices $(HJ - \gamma_i I)$ and $Z^\dagger J(HJ - \gamma_i I)Z = H' - \gamma_i J$ are equal, and the rank of the latter is, obviously, $2n-k$, the homogeneous system $(HJ - \gamma_i I)(x) = (0)$ has exactly $2n - (2n-k) = k$ independent solutions.

(d) The k independent eigenvectors $(x_1), \ldots, (x_k)$ belonging to the degenerate eigenvalue γ_i, can be made orthonormal (with respect to J) via the Schmidt process. Assume, for definiteness, $\gamma_i > 0$. Normalize (x_1) and denote the resulting vector by (y_1). Now subtract from (x_2) its component along (y_1), that is,

$$(x_2') = (x_2) - (y_1)^\dagger J(x_2)\cdot(y_1). \tag{33}$$

Clearly, $(x_2') \neq (0)$ [or else (x_2) and (y_1) would be linearly dependent], and $(x_2')^\dagger J(y_1) = 0$. Since (x_2') is also an eigenvector of HJ (with eigenvalue $\gamma_i > 0$), we have by (a), $(x_2')^\dagger J(x_2') > 0$. Normalize (x_2') and denote the resulting vector by (y_2). The process can be continued to obtain $(y_1), \ldots, (y_k)$ satisfying

$$HJ(y_l) = \gamma_i(y_l), \quad \text{and} \quad (y_l)^\dagger J(y_m) = \delta_{lm}. \tag{34}$$

(e) If $(x_i) = \begin{pmatrix}u_i\\ v_i\end{pmatrix}$ is an eigenvector of HJ with eigenvalue γ_i, then $(\hat{x}_i) = \begin{pmatrix}v_i^*\\ u_i^*\end{pmatrix}$ is an eigenvector of HJ with eigenvalue $-\gamma_i$. Indeed, using the explicit form

$$\begin{pmatrix}\alpha & -\beta\\ \beta^* & -\alpha^*\end{pmatrix}\begin{pmatrix}u_i\\ v_i\end{pmatrix}, = \gamma_i\begin{pmatrix}u_i\\ u_i\end{pmatrix},$$

the assertion is obvious. Since both γ_i and $-\gamma_i$ are eigenvalues,

$$\det(HJ - \gamma I) = \prod_{i=1}^{n}(\gamma^2 - \gamma_i^2). \tag{35}$$

We can now summarize the construction of the diagonalizing matrix $A^\dagger$.

(i) Find the n positive roots of the characteristic polynomial (35).

(ii) Obtain n independent eigenvectors $(x_1), \ldots, (x_n)$ belonging to the positive roots $\gamma_1, \ldots, \gamma_n$.

(iii) If necessary, use the Schmidt process to complete the orthonormalization, and denote the resulting vectors by (z_i). Thus, $(z_i)^\dagger J(z_j) = \delta_{ij}$.

(iv) The first half of $A^\dagger$, namely, $\binom{\lambda^\dagger}{\mu^\dagger}$ is given by

$$\binom{\lambda^\dagger}{\mu^\dagger} = ((z_1)\cdots(z_n)) \tag{36}$$

(v) Complete

$$A^\dagger = \begin{pmatrix} \lambda^\dagger & \tilde{\mu} \\ \mu^\dagger & \tilde{\lambda} \end{pmatrix} = ((z_1)\cdots(z_n)(\hat{z}_1)\cdots(\hat{z}_n)), \tag{37}$$

where $(\hat{z}_i) = \binom{v_i^*}{u_i^*}$ for $(z_i) = \binom{u_i}{v_i}$.

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APPENDIX

The purpose of the Appendix is to amend a shortcoming in a related work by the same author. In Ref. 2 the following problem is discussed: Given the diagonalizing matrix $A = \begin{pmatrix} \lambda & \mu \\ \mu^* & \lambda^* \end{pmatrix}$, find the transformation brackets connecting base states of the old operators $(a_i, a_i^\dagger)$ with those of the new operators $(b_i, b_i^\dagger)$. In order to evaluate a multidimentional normalization integral [Ref. 2, Eq. (76)], I have assumed, in addition to Eq. (5), the reality condition

$$(\lambda^\dagger\lambda) = (\lambda^\dagger\lambda)^*. \tag{A1}$$

It turned out that (A1) is too strong in the sense that it cannot always be met. Thus, for example, for $n=2$, the two matrices

$$\lambda = \begin{pmatrix} \alpha & -i\alpha \\ -i\beta & \beta \end{pmatrix} \quad \text{and} \quad \mu = \begin{pmatrix} a & ia \\ b & -ib \end{pmatrix},$$

with α, β, a, b real, and $\beta^2 \neq \alpha^2$, $a^2 = \alpha^2 - \frac{1}{2}$, and $b^2 = \beta^2 - \frac{1}{2}$, fulfill Conditions (5) but violate (A1). Now the normalization integral can be written as

$$\text{Integral} = \int \frac{d^{2n}x}{\pi^n} \exp[-(\tilde{x})F(x)], \tag{A2}$$

where

$$F = \begin{pmatrix} 1+\tau_R & \tau_I \\ \tau_I & 1-\tau_R \end{pmatrix} \tag{A3}$$

is a real $2n$ by $2n$ symmetric matrix, with

$$\tau_R = \mathrm{Re}(\lambda^{-1}\mu) \quad \text{and} \quad \tau_I = \mathrm{Im}(\lambda^{-1}\mu). \tag{A4}$$

Let Q be a real orthogonal matrix diagonalizing F, that is,

$$QF\tilde{Q} = f, \quad f_{ij} = \delta_{ij} f_i. \tag{A5}$$

Since the Jacobian of the transformation $(y) = Q(x)$ is equal to 1, the integral (A2) reduces to

$$\begin{aligned} \text{Integral} &= \int \frac{d^{2n}y}{\pi^n} \exp\left(-\sum_{i=1}^{2n} f_i y_i^2\right) = \prod_{i=1}^{2n} \frac{1}{\pi^{1/2}} \int e^{-f_i y_i^2} dy_i \\ &= \prod_{i=1}^{2n} f_i^{-1/2} = (\det F)^{-1/2}, \end{aligned} \tag{A6}$$

provided all the eigenvalues f_i are positive. We shall now show that this is indeed the case. Consider the matrix

$$G = F - I = \begin{pmatrix} \tau_R & \tau_I \\ \tau_I & -\tau_R \end{pmatrix}, \tag{A7}$$

with eigenvalues $g_i = f_i - 1$. The assertion will be established if $g_i^2 < 1$ for $i = 1, \ldots, 2n$. Let $\binom{x}{y}$ be a normalized eigenvector of G with eigenvalue g. Then

$$G^2\binom{x}{y} = \begin{pmatrix} B & C \\ -C & B \end{pmatrix}\binom{x}{y} = g^2\binom{x}{y}, \tag{A8}$$

where

$$B = \tau_R^2 + \tau_I^2 \quad \text{and} \quad C = \tau_R\tau_I - \tau_I\tau_R. \tag{A9}$$

But $(z) = (x) + i(y)$ also satisfies

$$\tau\tau^\dagger(z) = (B - iC)(z) = g^2(z), \tag{A10}$$

where

$$\tau = \tau_R + i\tau_I. \tag{A11}$$

Hence, by Eq. (5),

$$g^2 = (z)^\dagger\tau\tau^\dagger(z) = 1 - (z)^\dagger(\lambda^\dagger\lambda)^{-1}(z) < 1. \tag{A12}$$

The result (A6) is, therefore, always valid (when A exists), and should replace Eq. (80) of Ref. 2.

[1] C. Tsallis, J. Math. Phys. 19, 277 (1978).
[2] Y. Tikochinsky, J. Math. Phys. 19, 270 (1978).
[3] See, for example, M. Böcher, *Introduction to Higher Algebra* (Macmillan, New York, 1915), p. 144.