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Eigenvalue and Eigenfunction of *n*-Mode Boson Quadratic Hamiltonian

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By means of the linear quantum transformation (LQT) theory, a concise diagonalization approach for the *n*-mode boson quadratic Hamiltonian is given, and a general method to calculate the wave function is proposed.

1. INTRODUCTION

It is well known that in quantum statistics one can obtain the exact solution of the Hamiltonian only for a few simple systems because the general systems have a complicated Hamiltonian with multimode coupling. Generally speaking, it is quite difficult find to analytically the exact solution for a complicated Hamiltonian. The usual approach is to approximate this complicated Hamiltonian by a quadratic Hamiltonian using, e.g., the mean-field approximation, the random-phase approximation, or the Hatree–Fock approximation. Therefore, it is of fundamental and practical significance to find exact solutions for systems of quadratic Hamiltonians.

However, to the best of our knowledge, for a general multimode boson quadratic Hamiltonian, only the energy spectrum has been calculated analytically [1, 2], and the methods of diagonalization are quite complicated and lengthy; no one has given a general method to calculate the wave function for this system. In this paper, with the aid of linear quantum transformation (LQT) theory [3–9], we give a detailed solution including the energy spectrum and wave function.

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2. EIGENVALUE

Consider a general n-mode boson quadratic system whose Hamiltonian reads

$$\hat{H} = a^{+} \alpha a + \frac{1}{2} a^{+}\gamma\tilde{a}^{+} + \frac{1}{2} \tilde{a}\gamma^{+}a = \frac{1}{2} \Lambda N \Sigma_S \tilde{\Lambda} - \frac{1}{2} \operatorname{tr} \alpha \tag{1}$$

where α is an $n \times n$ Hermitian matrix, γ is an $n \times n$ complex symmetry matrix.

$$N = \begin{pmatrix} \alpha & -\gamma \\ \gamma^{*} & -\tilde{\alpha} \end{pmatrix}$$

is a “negative Hermitian” matrix [4] ($N^{-} = N$), and $\Lambda = (a^{+}, \tilde{a})$, $a^{+} = (a_1^{+}, a_2^{+}, \ldots, a_n^{+})$, and $\tilde{a} = (a_1, a_2, \ldots, a_n)$, where a_i^{+} and a_i are, respectively, ith boson creation and annihilation operators in n-mode Fock space, and the operator Λ satisfies the commutation relation $[\tilde{\Lambda}_i, \Lambda_j] = (\Sigma_B^{-1})_{ij}$, $\Sigma_B = \begin{pmatrix} 0 & -I \\ I & 0 \end{pmatrix}$.

Consider the following quantum transformation:

$$\Lambda' = U^{-1}\Lambda U = \Lambda M = \Lambda \begin{pmatrix} U & V^{*} \\ V & U^{*} \end{pmatrix} \tag{2}$$

where $M \in C^{2n\times 2n}$ and it should obey the following sympletic relation [8]:

$$M\Sigma_B\tilde{M} = \Sigma_B \tag{3}$$

If the operator U is the unitary operator, the matrix M is the “negative unitary” matrix [4] ($M^{-} = M^{-1}$). Because of Eq. (3), the commutation relation will be automatically preserved after the transformation, i.e., $[\tilde{\Lambda}_i', \Lambda'^{j}] = (\Sigma_B^{-1})_{ij}$.

From Eq. (2), we have

$$\Lambda = \Lambda' M^{-1} \tag{4}$$

Substituting Eq. (4) into Eq. (1) and noting Eq. (3), we can rewrite the Hamiltonian as

$$\hat{H} = \frac{1}{2} \Lambda' M^{-1} N\Sigma_B\tilde{M}^{-1}\tilde{\Lambda}' - \frac{1}{2} \operatorname{tr} \alpha = \frac{1}{2} \Lambda' M^{-1}NM \Sigma_B\tilde{\Lambda}' - \frac{1}{2} \operatorname{tr} \alpha \tag{5}$$

It can be verified that if the $2n \times 2n$ “negative Hermitian” matrix N is positive-definite, the matrix N can be diagonalized by the “negative unitary” matrix M (see Appendix), i.e.,

$$M^{-1}NM = \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix}, \qquad \Omega = \begin{pmatrix} \lambda_1 & & 0 \\ & \lambda_2 & \\ & & \ddots \\ 0 & & \lambda_n \end{pmatrix} \tag{6}$$

where $\lambda_i > 0$ ($i = 1, 2, \ldots, n$) and can be calculated from the following equation:

$$\det\begin{pmatrix} \alpha - \lambda & -\gamma \\ \gamma^* & -\tilde{\alpha} - \lambda \end{pmatrix} = 0$$

Thus we obtain the diagonalized Hamiltonian, its energy spectrum, and eigenstates in quasiparticle representation:

$$\tilde{H} = \sum_{i=1}^{n} \lambda_l \left(a_i'^{+} a_i' + \frac{1}{2} \right) - \frac{1}{2} \operatorname{tr} \alpha \tag{7}$$

$$E_{n_1, n_2, \ldots, n_n} = \sum_{i=1}^{n} \lambda_i \left(n_l + \frac{1}{2} \right) - \frac{1}{2} \operatorname{tr} \alpha \tag{8}$$

$$|n\rangle' = |n_1, n_2, \ldots, n_n\rangle' = \prod_{i=1}^{n} \frac{(a_i'^{+})^{n_i}}{\sqrt{n_i!}} |0\rangle' \tag{9}$$

3. EIGENFUNCTION

Now let us calculate the eigenfunction of the Hamiltonian,

$$\Psi_{n_1, n_2, \ldots, n_n}(q) = \langle q | n \rangle = \langle q | U^{-1} | n \rangle' \tag{10}$$

where U is the unitary operator of transformation, and the antinormal order product of U^{-1} can be calculated from refs. 7 and 8:

$$U^{-1} = [\det U^*]^{-1/2} \, {}^{+}_{+} \exp\left\{ \frac{1}{2} \Lambda \begin{pmatrix} V^* U^{*-1} & 1 - U^{+-1} \\ 1 - U^{*-1} & -\tilde{V} U^{+-1} \end{pmatrix} \tilde{\Lambda} \right\}^{+}_{+} \tag{11}$$

where the ${}^{+}_{+} \ldots {}^{+}_{+}$ denotes the antinormal order product, while $|q\rangle = |q_1, q_2, \ldots, q_n\rangle$ is the eigenstate in the coordinate representation:

$$\langle q| = \langle 0| \pi^{-n/4} \exp\left[-\frac{\tilde{q} q}{2} - \frac{\tilde{a} a}{2} + \sqrt{2} \tilde{a} q \right] \tag{12}$$

By Eq. (10) of ref. 10, substituting the Eqs. (9), (11), and (12) into Eq. (10), we can immediately write the $\Psi(q)$ as follows:

$$\Psi(q) = \pi^{-n/4} \exp\left(-\frac{\tilde{q}q}{2}\right)\left[\det U^* \cdot \det\begin{pmatrix} U^{*-1} & 1 + \tilde{V}U^{+-1} \\ -U^{+-1}V^{+} & U^{+-1} \end{pmatrix}\right]^{-1/2}$$
$$\times \prod_{i=1}^{n} \frac{1}{\sqrt{n_l!}} \left(\frac{d}{d\beta_l}\right)^{n_i} \exp\left\{\frac{1}{2}(\tilde{\beta}, \tilde{\beta}')\begin{pmatrix} -U^{+-1}V^{+} & U^{+-1} \\ U^{*-1} & 1 + \tilde{V}U^{+-1} \end{pmatrix}^{-1}\begin{pmatrix} \beta \\ \beta' \end{pmatrix}\right\}_{\beta=0} \tag{13}$$

where $\beta' = \sqrt{2}q$, $\tilde{q} = (q_1, q_2, \ldots, q_n)$.

Using the sympletic relation (3) and the formula [2]

$$\begin{pmatrix} A & B \\ C & D \end{pmatrix}^{-1} = \begin{pmatrix} (A - BD^{-1}C)^{-1} & -(A - BD^{-1}C)^{-1}BD^{-1} \\ -(D - CA^{-1}B)^{-1}CA^{-1} & (D - CA^{-1}B)^{-1} \end{pmatrix}$$

$$\det\begin{pmatrix} A & B \\ C & D \end{pmatrix} = \det A \cdot \det(D - CA^{-1}B)$$

where A, B, C, and D are $n \times n$ matrices, we can derive

$$\begin{pmatrix} -U^{+-1}V^{+} & U^{+-1} \\ U^{*-1} & 1 + \tilde{V}U^{+-1} \end{pmatrix}^{-1} = \begin{pmatrix} -A_1 & A_2 \\ \tilde{A}_2 & A_3 \end{pmatrix} \tag{14}$$

where

$$\left.\begin{aligned} A_1 &= U^*[V^* + (U^+ + \tilde{V})^{-1}]^{-1} = \tilde{A}_1 \\ A_2 &= (V^+ + \tilde{U})^{-1} \\ A_3 &= U^+[U^+ + \tilde{V} + V^{*-1})]^{-1} = \tilde{A}_3 \end{aligned}\right\} \tag{15}$$

$$\det\begin{pmatrix} U^{*-1} & 1 + \tilde{V}U^{+-1} \\ -U^{+-1}V^{+} & U^{+-1} \end{pmatrix} = (\det U^{*-1})^2 \cdot \det[1 + (V^{+}U^* + V^{+}V)] \tag{16}$$

Using Eq. (14), we have

$$\exp\left\{\frac{1}{2}(\tilde{\beta}, \tilde{\beta}')\begin{pmatrix} -U^{+-1}V^{+} & U^{+-1} \\ U^{*-1} & 1 + \tilde{V}U^{+-1} \end{pmatrix}^{-1}\begin{pmatrix} \beta \\ \beta' \end{pmatrix}\right\}$$
$$= \exp\left\{\frac{1}{2}(\tilde{\beta}, \tilde{\beta}')\begin{pmatrix} -A_1 & A_2 \\ \tilde{A}_2 & A_3 \end{pmatrix}^{-1}\begin{pmatrix} \beta \\ \beta' \end{pmatrix}\right\}$$
$$= \exp\left(\frac{1}{2}\tilde{\beta}'A_3\beta'\right) \cdot \exp\left(\frac{1}{2}\tilde{\beta}\tilde{D}D\beta'\right) \cdot \exp\left[-\sum_i (\alpha_i - \delta_i)^2\right] \tag{17}$$

where

$$\tilde{D} = \tilde{A}_2 \cdot A_1^{-1/2}, \qquad \alpha_i = \frac{1}{\sqrt{2}} \sum_k \beta_k (A_1^{1/2})_{ki}, \qquad \delta_i = \sum_j q_j \, \tilde{D}_{ji} \tag{18}$$

Note

$$\prod_i^n d\alpha_i = \frac{1}{\sqrt{2}} \sqrt{\det A_i} \prod_i^n d\beta_i \tag{19}$$

Substituting Eqs. (16), (17), and (19) into Eq. (13), we have

$$\begin{aligned}
\Psi(q) = \pi^{-n/4} \exp\left(-\frac{\tilde{q}q}{2}\right) &\left\{\frac{\det U^*}{\det[1 + (V^+U^* + V^+V)]}\right\}^{1/2} \\
&\times \prod_{i=1}^n (2^{n_i} n_i!)^{-1/2} (\det A_1)^{n_i/2} \exp\left(\frac{1}{2} \tilde{\beta}' A_3 \beta'\right) \\
&\times \exp\left(\frac{1}{2} \tilde{\beta}' \tilde{D} D \beta'\right) \left(\frac{d}{d\alpha_i}\right)^{n_i} \left\{\exp\left[-\sum_i (\alpha_i - \delta_i)^2\right]\right\}_{\alpha=0}
\end{aligned} \tag{20}$$

Using the formula

$$\left(\frac{d}{dx}\right)^n e^{-x^2} = (-1)^n \, e^{-x^2} H_n(x)$$

we can get the eigenfunction as follows:

$$\begin{aligned}
\Psi(q) &= \left\{\frac{\det U^*}{\det[1 + (V^+U^* + V^+V)]}\right\}^{1/2} \prod_i^n [2^{n_i} n_i! \, \pi^{-n/2} (\det A_i)^{-n_i}]^{-1/2} \\
&\quad \times \exp\left[-\tilde{q}\left(-A_3 + \frac{1}{2}\right) q\right\} H_{n_i}\left(\sum_k q_k (A_2 A_1^{-1/2})^{ki}\right) \\
&= \left\{\frac{\det U^*}{\det[1 + (V^+U^* + V^+V]}\right\}^{1/2} \prod_i^n [2^{n_i} n_i! \, \pi^{-n/2} (\det A_1)^{-n_i}]^{-1/2} \\
&\quad \times \exp\left\{\left[\sum_k q_k (A_3^{1/2})_{ki}\right]^2 - \frac{1}{2} q^2\right\} \times H_{n_i}\left(\sum_k q_k (A_2 A_1^{-1/2})_{ki}\right)
\end{aligned} \tag{21}$$

In summary, as discussed above, we clearly see that this approach of calculating the eigenfunction is general. We point out that, for a general *n*-mode boson quadratic Hamiltonian, other methods to calculate the eigenfunction are quite complicated and lengthy.

APPENDIX

Theorem. If a negative Hermitian matrix N is positive-definite, one can find a negative unitary matrix M to diagonalize it to the following form

$$M^{-1}NM = \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix}, \qquad \Omega = \begin{pmatrix} \lambda_1 & & & 0 \\ & \lambda_2 & & \\ & & \ddots & \\ 0 & & & \lambda_h \end{pmatrix} \tag{A1}$$

Proof. From ref. 8, we know that if the $2n \times 2n$ negative Hermitian matrix N is positive-definite, then it will not have any zero root, and all of the $2n$ characteristic roots λ_i are real and make up n pairs $\pm \lambda_i$ ($i = 1, 2, \ldots, n$). The corresponding eigenvectors are $\{|\alpha_i\rangle, |\beta_i\rangle\}$, where

$$N|\alpha\rangle = \lambda|\alpha\rangle, \qquad N|\beta\rangle = -\lambda|\beta\rangle \tag{A2}$$

and satisfy the following orthogonal relations:

$$\langle\alpha_{l'}|\Sigma|\alpha_l\rangle = \delta_{ll'}, \qquad \langle\beta_l|\Sigma|\beta_{l'}\rangle = -\delta_{ll'} \tag{A3}$$
$$\langle\alpha_{l'}|\Sigma|\beta_l\rangle = 0, \qquad \Sigma = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}$$

We can construct the M in the following way:

$$M = (|\alpha_1\rangle, |\alpha_2\rangle, \ldots, |\alpha_n\rangle; |\beta_1, |\beta_2\rangle, \ldots, |\beta_n\rangle) \tag{A4}$$

and its inverse matrix reads

$$M^{-1} = \Sigma \begin{pmatrix} \langle\alpha_1| \\ \langle\alpha_2| \\ \vdots \\ \langle\alpha_n| \\ \langle\beta_1| \\ \langle\beta_2| \\ \vdots \\ \langle\beta_n| \end{pmatrix} \Sigma = \Sigma\, M^{+}\, \Sigma = M^{-} \tag{A5}$$

Obviously, the above matrix M is a "negative unitary" matrix. From Eqs. (A4) and (A2), it is easy to show that

$$M^{-1}NM = \begin{pmatrix} \lambda_1 & & & & & & 0 \\ & \lambda_2 & & & & & \\ & & \ddots & & & & \\ & & & \lambda_n & & & \\ & & & & -\lambda_1 & & \\ & 0 & & & & \ddots & \\ & & & & & & -\lambda_n \end{pmatrix} = \begin{pmatrix} \Omega & 0 \\ 0 & -\Omega \end{pmatrix} \tag{A6}$$

If we denote

$$|\alpha_l\rangle = \begin{pmatrix} X_l \\ Y_l \end{pmatrix}, \qquad |\beta_l\rangle = \begin{pmatrix} Y_l^* \\ X_l^* \end{pmatrix}, \qquad \langle\alpha_l| = (X_l^+, Y_l^+), \qquad \langle\beta_l| = (\tilde{Y}_l, \tilde{X}_l)$$

where

$$X_l = \begin{pmatrix} x_1^{(l)} \\ x_2^{(l)} \\ \vdots \\ x_n^{(l)} \end{pmatrix}, \qquad Y_l = \begin{pmatrix} y_1^{(l)} \\ y_2^{(l)} \\ \vdots \\ y_n^{(l)} \end{pmatrix}$$

we can rewrite the matrix *M* as

$$M = \begin{pmatrix} X & Y^* \\ Y & X^* \end{pmatrix} \tag{A7}$$

Furthermore, we can verify that this matrix *M* satisfies the sympletic condition (5). On one hand, from Eq. (A7) we have

$$\tilde{M}\,\Sigma_B\,M = \begin{pmatrix} \tilde{X}Y - \tilde{Y}X & \tilde{X}X^* - \tilde{Y}Y^* \\ Y^+Y - X^+X & Y^+X^* - X^+Y^* \end{pmatrix} \tag{A8}$$

On the other hand, from Eq. (A3) we have

$$(X^+, Y^+)\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = X^+X - Y^+Y = 1, \tag{A9}$$

$$(\tilde{Y}, \tilde{X})\begin{pmatrix} 1 & 0 \\ 0 & - \end{pmatrix}\begin{pmatrix} X \\ Y \end{pmatrix} = \tilde{Y}X - \tilde{X}Y = 0$$

Substituting Eq. (A9) into Eq. (A8), we get the sympletic relation (3).

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