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ENERGY SPECTRUM AND WAVE FUNCTION FOR MULTI-MODE COUPLED NON-IDENTICAL HARMONIC OSCILLATORS

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By means of the linear quantum transformation theory, we consisely derive the exact solution including energy spectrum and wave function for multi-mode coupled non-identical harmonic oscillators.

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I. INTRODUCTION

It is well known that many physical problems in various fields (for example, in quantum statistics, atomic physics, and nuclear physics and quantum chemistry.) are related to the coupled harmonic oscillators. So, it is important to study the exact solution for such problems. However, it has been only given the solution for coupled identical harmonic oscillators in previous work.[1—5] In fact, we often need to copy with the following coupled non-identical oscillator, whose Hamiltonian reads

$$\widehat{H}=\sum_{i=1}^{n}\left(\frac{1}{2m_i}\hat{p}_i^2+\frac{1}{2}m_i\omega_i^2\hat{x}_i^2\right)+\frac{1}{2}\sum_{i=1}^{n}k_{ij}\hat{x}_i\hat{x}_j\,, \quad (1)$$

where $k_{ij}=k_{ji}$, m_i and ω_i stand for mass and frequency respectively.

So far as we know, the above Hamiltonian has not been discussed in detail. In this paper, with the help of linear quantum transformation (LQT) theory, we shall give all detailed solutions of the system, i.e., the energy spectrum, the wave function, and the unitary operator for diagonalizing the systme. One may see, from the following derivation, the advantages and universality of the LQT theory.

II. QUANTUM TRANSFORMATION OF DIAGONALIZATION

For the sake of convenience, we first take the dimensionless transformation

$$\widehat{Q}_i=\sqrt{\frac{m_i\omega_i}{\hbar}}\hat{x}_i, \quad \widehat{P}_i=\sqrt{\frac{1}{m_i\omega_i\hbar}}\hat{p}_i\,,$$

where operators $\widehat{Q}_i$ and $\widehat{P}_i$ satisfy the commutation rules

$$\left[\widehat{Q}_i,\widehat{P}_j\right]=\mathrm{i}\delta_{ij}\,. \quad (2)$$

Thus, Eq.(1) becomes

$$\begin{aligned}\widehat{H}&=\sum_{i=1}^{n}\frac{1}{2}\hbar\omega_i(\widehat{P}_i^2+\widehat{Q}_i^2)+\frac{1}{2}\hbar\sum_{i,j=1}^{n}k'_{ij}\widehat{Q}_i\widehat{Q}_j\\&=\frac{1}{2}(\widehat{Q},\widehat{P})\begin{pmatrix}A&0\\0&\Omega\end{pmatrix}\begin{pmatrix}\widetilde{\widehat{Q}}\\\widetilde{\widehat{P}}\end{pmatrix}, \quad (3)\end{aligned}$$

where

$$A=K'+\Omega=\widetilde{A}, \quad \Omega=\begin{pmatrix}\omega_1&&&0\\&\omega_2&&\\&&\ddots&\\0&&&\omega_n\end{pmatrix},$$

$$\widehat{Q}=(\widehat{Q}_1,\widehat{Q}_2,\cdots,\widehat{Q}_n), \quad \widehat{P}=(\widehat{P}_1,\widehat{P}_2,\cdots,\widehat{P}_n)\,.$$

To simplfy, we have let $\hbar=1$.

Now, consider the following quantum transformation

$$(\widehat{Q}',\widehat{P}')=(\widehat{Q},\widehat{P})M=(\widehat{Q},\widehat{P})\begin{pmatrix}\Omega^{-1/2}B&0\\0&\Omega^{1/2}B\end{pmatrix}, \quad (4)$$

where B is a real $n\times n$ orthogonal matrix, i.e., $\widetilde{B}=B^{-1}$, while $M\in R^{n\times n}$ and M should obey the following symplistic relation[6,7]

$$M\Sigma_B\widetilde{M}=\Sigma_B, \quad \Sigma_B=\begin{pmatrix}0&I\\-I&0\end{pmatrix}. \quad (5)$$

In view of the symplistic relation, the commutation rules are preserved after transformation, i.e., $[\widehat{Q}'_i,\widehat{P}'_j]=[\widehat{Q}_i,\widehat{P}_j]=\mathrm{i}\delta_{ij}$.

From Eq.(4), we have

$$\begin{aligned}\left(\widehat{Q},\widehat{P}\right) &= \left(\widehat{Q}',\widehat{P}'\right)M^{-1} \\ &= \left(\widehat{Q}',\widehat{P}'\right)\begin{pmatrix} B^{-1}\Omega^{1/2} & 0 \\ 0 & B^{-1}\Omega^{-1/2}\end{pmatrix}. \quad (6)\end{aligned}$$

Substituting Eq.(6) into Eq.(3), the Hamiltonian can be written as

$$\begin{aligned}\widehat{H} &= \frac{1}{2}\left(\widehat{Q}',\widehat{P}'\right)\begin{pmatrix} B^{-1}\Omega^{1/2} & 0 \\ 0 & B^{-1}\Omega^{1/2}\end{pmatrix}\begin{pmatrix} K+\Omega & 0 \\ 0 & \Omega\end{pmatrix} \\ &\quad \begin{pmatrix} \Omega^{1/2}\widetilde{B}^{-1} & 0 \\ 0 & \Omega^{-1/2}\widetilde{B}^{-1}\end{pmatrix}\begin{pmatrix}\widetilde{\widehat{Q}} \\ \widetilde{\widehat{P}}\end{pmatrix} \\ &= \frac{1}{2}\left(\widehat{Q}',\widehat{P}'\right)\begin{pmatrix} B^{-1}A'B & 0 \\ 0 & I\end{pmatrix}\begin{pmatrix}\widetilde{\widehat{Q}}' \\ \widetilde{\widehat{P}}'\end{pmatrix}, \quad (7)\end{aligned}$$

where $A' = \Omega^{1/2}A\Omega^{-1/2} = \widetilde{A}'$.

It is known that, in general linear algebraic theory, an arbitrary real symmetrical matrix can be certainly diagonalized by a full-rank orthogonal matrix. Therefore, we have

$$B^{-1}A'B = \Lambda = \mathrm{diag}(\lambda_1,\lambda_2,\cdots,\lambda_n)\,.$$

Thus we obtain the diagonalized Hamiltonian

$$\begin{aligned}\widehat{H} &= \frac{1}{2}\left(\widehat{Q}',\widehat{P}'\right)\begin{pmatrix}\Lambda & 0 \\ 0 & I\end{pmatrix}\begin{pmatrix}\widetilde{\widehat{Q}}' \\ \widetilde{\widehat{P}}'\end{pmatrix} \\ &= \sum_{i=1}^{n}\left[\frac{1}{2}\lambda_i\left(\widehat{Q}_i'\right)^2 + \frac{1}{2}\left(\widehat{P}_i'\right)^2\right]. \quad (8)\end{aligned}$$

In the following discussion, we shall consider two cases. One is that matrix A' is the positive definite symmetrical matrix, and the other is that it is the semi-positive definite one.

In the first case, the matrix A' has no zero character roots, so Eq.(8) can be written as

$$\begin{aligned}\widehat{H} &= \frac{1}{2}\sum_{i=1}^{n}\sqrt{\lambda_i}\left(\sqrt{\lambda_i}\widehat{Q}_i'^2 + \widehat{P}_i'^2/\sqrt{\lambda_i}\right) \\ &= \frac{1}{2}\sum_{i=1}^{n}\sqrt{\lambda_i}\left(\widehat{Q}_i''^2 + \widehat{P}_i''^2\right), \quad (9)\end{aligned}$$

where

$$\left(\widetilde{\widehat{Q}}'',\widetilde{\widehat{P}}''\right) = \left(\widetilde{\widehat{Q}}',\widetilde{\widehat{P}}'\right)M' = \left(\widetilde{\widehat{Q}}',\widetilde{\widehat{P}}'\right)\begin{pmatrix}\Lambda^{1/4} & 0 \\ 0 & \Lambda^{-1/4}\end{pmatrix}. \quad (10)$$

If we use the following formula

$$\left(a'^{+},\widetilde{a}'\right) = \left(\widehat{Q}'',\widehat{P}''\right)N = \left(\widehat{Q}'',\widehat{P}''\right)\begin{pmatrix} \frac{I}{\sqrt{2}} & \frac{I}{\sqrt{2}} \\ -\mathrm{i}\frac{I}{\sqrt{2}} & \mathrm{i}\frac{I}{\sqrt{2}}\end{pmatrix}, \quad (11)$$

where N is the unitary matrix, we have

$$\widehat{H} = \sum_{i=1}^{n}\left(a_i'^{+}a_i' + \frac{1}{2}\right)\overline{\omega}_i \qquad \overline{\omega}_i = \sqrt{\lambda_i}\,, \quad (12)$$

where $a_i'^{+}$ and a_i' are quasi-particle creation and annihilation operators, respectively; and they satisfy the commutation rules: $[a_i'^{+}, a_j'] = \delta_{ij}$.

If matrix A' is a semi-positive definite matrix, it has some zero character roots. Assuming there are K zero roots among n roots λ_i, Eq.(8) can be written as

$$\widehat{H} = \sum_{i=1}^{n-k}\frac{1}{2}\sqrt{\lambda_i}\left(\left(\widehat{Q}_i''\right)^2 + \left(\widehat{P}_i''\right)^2\right) + \frac{1}{2}\sum_{j=1}^{k}\left(\widehat{P}_j'\right)^2. \quad (13)$$

Obviously, the second term on the right of Eq.(13) stands for free motion. Therefore, the system has not only a discrete energy spectrum, but also a continuous energy spectrum.

Similarly, in the Fock space, Eq.(13) can be rewritten as

$$\begin{aligned}\widehat{H} &= \sum_{i=1}^{n-k}\left(a_i'^{+}a_i' + \frac{1}{2}\right)\overline{\omega}_i + \frac{1}{2}\sum_{j=1}^{k}\left(\widehat{P}_j'\right)^2, \\ E &= E_{n_1,n_2,\cdots,n_{n-k}} + E_p = \sum_{i=1}^{n-k}\left(n_i + \frac{1}{2}\right)\overline{\omega}_i + \frac{1}{2}P''^2, \\ P''^2 &= \sum_{j=1}^{k}\left(P_j''\right)^2. \quad (14)\end{aligned}$$

III. UNITARY OPERATOR FOR DIAGONALIZATION

For the sake of convenience, we just consider the system of which the Hamiltonian is positive definite, i.e., matrix A' is a positive definite matrix.

From Eqs.(4) and (10), we have

$$\begin{aligned}\left(\widehat{Q}'',\widehat{P}''\right) &= \left(\widehat{Q}',\widehat{P}'\right)M' = \left(\widehat{Q},\widehat{P}\right)MM' \\ &= \left(\widehat{Q},\widehat{P}\right)\begin{pmatrix} B' & 0 \\ 0 & \widetilde{B}'^{-1}\end{pmatrix}, \quad (15)\end{aligned}$$

where $B' = \Omega^{-1/2}B\Lambda^{1/4}$. Now, we calculate the unitary operator generating the transformation, Eq.(15).

Evidently

$$\left(\widehat{Q}'', \widehat{P}''\right) = U^{-1}\left(\widehat{Q}, \widehat{P}\right)U = \left(\widehat{Q}, \widehat{P}\right)\begin{pmatrix} B' & 0 \\ 0 & \widetilde{B}'^{-1} \end{pmatrix}. \tag{16}$$

From Eq.(16), we know

$$U|q\rangle = \sqrt{\det B'}|qB'\rangle\,, \tag{17}$$

where $|q\rangle = |q_1, q_2, \cdots, q_n\rangle = \prod_{i=1}^{n}|q_i\rangle$ is the position eigenstate in coordinate space. In fact, it is easy to prove that Eq.(17) satisfies Eq.(16).

Proof:

$$\begin{aligned} U^{-1}\widehat{Q}U|q\rangle &= U^{-1}\widehat{Q}\sqrt{\det B'}|qB'\rangle \\ &= U^{-1}qB'\sqrt{\det B'}|qB'\rangle = qB'|q\rangle = \widehat{Q}B'|q\rangle, \\ U^{-1}\widehat{Q}U &= \widehat{Q}B'\,. \end{aligned}$$

Similarly,

$$U^{-1}\widehat{P}U = \widehat{P}\widetilde{B}'^{-1}\,.$$

Therefore, we have

$$U^{-1}\left(\widehat{Q}, \widehat{P}\right)U = \left(\widehat{Q}, \widehat{P}\right)\begin{pmatrix} B' & 0 \\ 0 & \widetilde{B}'^{-1} \end{pmatrix}. \tag{18}$$

The proof is completed.

Obviously, it is also necessary to prove that the operator U is the unitary operator.

$$\begin{aligned} UU^{+} &= \int U|q\rangle\langle q|U^{+}\mathrm{d}^n q \\ &= \det B' \int |qB'\rangle\langle qB'|\mathrm{d}^n q = 1\,, \\ U^{+}U &= \int U^{+}|q\rangle\langle q|U\mathrm{d}^n q \\ &= \frac{1}{\det B'}\int |qB'^{-1}\rangle\langle qB'^{-1}|\mathrm{d}^n q = 1\,, \\ U^{+} &= U^{-1}\,. \end{aligned}$$

From Eq.(11) and the following formula

$$\left(a^{+}, \widetilde{a}\right) = \left(\widehat{Q}, \widetilde{P}\right)N\,, \tag{19}$$

we easily see that it is the same unitary operator U that generates not only transformation Eq.(16), but also the following transformation:

$$\left(a'^{+}, \widetilde{a}'\right) = U^{-1}\left(a^{+}, \widetilde{a}\right)U = \left(a^{+}, \widetilde{a}\right)T\,, \tag{20}$$

where

$$T = \begin{pmatrix} \frac{1}{2}\left(B' + \widetilde{B}'^{-1}\right) & \frac{1}{2}\left(B' - \widetilde{B}'^{-1}\right) \\ \frac{1}{2}\left(B' - \widetilde{B}'^{-1}\right) & \frac{1}{2}\left(B' + \widetilde{B}'^{-1}\right) \end{pmatrix} = \begin{pmatrix} X & Y \\ Y & X \end{pmatrix}. \tag{21}$$

Now, from Refs.[9] and [10], we can immediately get the explicit expression of unitary operator U:

$$U^{+} = U^{-1} = [\det X]^{-1/2} : \exp\left\{\frac{1}{2}\left(a^{+}, \widetilde{a}\right)\begin{pmatrix} -YX^{-1} & \widetilde{X}^{-1} - 1 \\ X^{-1} - 1 & \widetilde{Y}X^{-1} \end{pmatrix}\begin{pmatrix} \widetilde{a}^{+} \\ a \end{pmatrix}\right\} : \,. \tag{22}$$

IV. WAVE FUNCTION IN COORDINATE REPRESENTATION

Now, let us calculate the wave function in the case that the system's Hamiltonian is positive. In this case, from Eq.(11), we get

$$|n_1, n_2, \cdots, n_n\rangle' = \frac{\left(a_1'^{+}\right)^{n_1}}{\sqrt{n_1!}}\frac{\left(a_2'^{+}\right)^{n_2}}{\sqrt{n_2!}}\cdots\frac{\left(a_n'^{+}\right)^{n_n}}{\sqrt{n_n!}}|0\rangle'. \tag{23}$$

From Eq.(17), we have

$$U^{-1}|q\rangle = \frac{1}{\sqrt{\det B'}}|qB'^{-1}\rangle\,. \tag{24}$$

Using the formula given above, we can easily get the wave function in coordinate representation:

$$\psi_{n_1,n_2,\cdots,n_n}(q) = \langle q|n_1, n_2, \cdots, n_n\rangle = \langle q|U|n_1, n_2, \cdots, n_n\rangle' = \langle qB'^{-1}|\frac{\left(a_1'^{+}\right)^{n_1}}{\sqrt{n_1!}}\frac{\left(a_2'^{+}\right)^{n_2}}{\sqrt{n_2!}}\cdots\frac{\left(a_n'^{+}\right)^{n_n}}{\sqrt{n_n!}}|0\rangle'\cdot\frac{1}{\sqrt{\det B'}}$$

$$= \frac{1}{\sqrt{\det B'}}\prod_{i=1}^{n}\left(\frac{m_i\omega_i}{\pi\hbar}\right)^{1/4}(2^{n_i}n_i!)^{-1/2}\exp\left\{-\left(\sum_k q_k B'^{-1}_{ki}\right)^2\right\}H_{n_i}\left(\sum_k q_k B'^{-1}_{ki}\right). \tag{25}$$

From the above discussion, we can again see that our approach is not only general but also direct and simple.

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