On Diagonalisation and Bound State Existence Conditions for Coupled Harmonic Oscillators

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Outline

Motivation

- Quadratic (Harmonic) Hamiltonian plays a unique role when it comes to the history of quantum physics since its inception.
- The range of applicability of the harmonic Hamiltonian is huge.
- Applications can be found in quantum physics, non-linear physics and biophysics to name a few.
- The diagonalisation methods for 3 coupled quantum harmonic oscillators (CQHO) in Merdaci and Jellal [Phys. Lett. A **384**, 126134 (2020) [arXiv:1909.01997 [quant-ph]]] and in Hassoul et. al. [Physica A: Statistical Mechanics and its Applications **604**, 127755 (2022)] are different approaches but used for the similar type of problem.
- It is desirable to find the connection between these two different methods to get more insights into the diagonalisation and then establish which one is more suitable for the problem of 3 coupled quantum harmonic oscillators.

Motivation

- In addition, the establishing of connection between two methods clearly explains some of the issues raised recently by Rahma et. al. [arXiv:2209.11560 [quant-ph]] on Hassoul et. al. especially related to the transformation matrix $\mathbb{R}$.
- Moreover, in the literature, many approaches have been developed for solving time-dependent and independent 3 CQHO problems.
- However, the studies have not specified the conditions and constraints that the model parameters should obey for the existence of bound state solutions.
- One of the major outcome of this work is to bridge this gap in the literature by deriving the necessary and sufficient conditions for time-dependent 3 CQHO that make sure the existence of bound states.

Two Diagonalisation Methods for Three Coupled Harmonic Oscillators

1. Diagonlisation by SU(3) Lie Group Structure

The main results of the time-dependent version of Merdaci and Jellal Hamiltonian diagonalised by using SU(3) group representation approach can be summarized as follows

$$
\begin{aligned}
H_1(t) &= \frac{1}{2}\Big(\frac{p_1^2}{m_1(t)} + \frac{p_2^2}{m_2(t)} + \frac{p_3^2}{m_3(t)} + m_1 w_1^2(t) x_1^2 + m_2 w_2^2(t) x_2^2 \\
&+ m_3 w_3^2(t) x_3^2 + D_{12}(t) x_1 x_2 + D_{13}(t) x_1 x_3 + D_{23}(t) x_2 x_3\Big). \quad (1)
\end{aligned}
$$

Where $(m_1(t), m_2(t), m_3(t))$, $(w_1(t), w_2(t), w_3(t))$ and $(D_{12}(t), D_{13}(t), D_{23}(t))$ are the different masses, frequencies and couplings of the three time-dependent CHO respectively.

After Rescaling

Eqn.(1) can be written as

$$\begin{aligned} H_2(t) &= \frac{1}{2m(t)}(p_1^2+p_2^2+p_3^2)+\frac{m(t)}{2}(w_1^2(t)X_1^2+w_2^2(t)X_2^2+w_3^2(t)X_3^2) \\ &+ m(J_{12}(t)X_1X_2+J_{13}(t)X_1X_3+J_{23}(t)X_2X_3) \end{aligned} \quad (2)$$

when one does rescaling of the variables in phase space

$$\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} \mu_1^{-1}(t)X_1 \\ \mu_2^{-1}(t)X_2 \\ \mu_3^{-1}(t)X_3 \end{pmatrix}, \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix} = \begin{pmatrix} \mu_1(t)P_1 \\ \mu_2(t)P_2 \\ \mu_3(t)P_3 \end{pmatrix} \quad (3)$$

here the model parameters are given as

$$\begin{aligned} m(t) &= (m_1(t)m_2(t)m_3(t))^{\frac{1}{3}},\ \mu_3(t)=(\frac{m_i(t)}{m(t)})^{\frac{1}{2}},\ \mu_1(t)\mu_2(t)\mu_3(t)=1, \\ J_{ij}(t) &= \frac{D_{ij}(t)}{2\sqrt{m_i(t)m_j(t)}} \end{aligned} \quad (4)$$

with the indices $i,j=1,2,3$.

Recasting

Then the Hamiltonian (2) was then cast in the following matrix form

$$H_2(t) = \frac{1}{2m(t)} \sum_{i,j=1}^{3} P_i \delta_{ij} P_j + \frac{1}{2m(t)} \sum_{i,j=1}^{3} X_i R_{ij}(t) X_j \quad (5)$$

here the two matrices R_{ij} and X are

$$R_{ij}(t) = \begin{pmatrix} w_1^2(t) & J_{12}(t) & J_{13}(t) \\ J_{12}(t) & w_2^2(t) & J_{23}(t) \\ J_{13}(t) & J_{23}(t) & w_3^2(t) \end{pmatrix}, X = \begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} \quad (6)$$

After this, a faithful representation of a matrix for diagonalising the Hamiltonian (5) introduced by generators of SU(3) lie group structure as follows

$$R_{ij}(t) = J_{12}(t)\lambda_1 + J_{13}(t)\lambda_4 + J_{23}(t)\lambda_6 + diag(w_1^2(t), w_2^2(t), w_3^2(t)) \quad (7)$$

Rotation by 3 angles

Rotation was made by 3 angles (φ, ϕ, θ), then,

$$\begin{pmatrix} X_1 \\ X_2 \\ X_3 \end{pmatrix} = M \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}, \begin{pmatrix} P_1 \\ P_2 \\ P_3 \end{pmatrix} = M \begin{pmatrix} \tilde{P}_1 \\ \tilde{P}_2 \\ \tilde{P}_3 \end{pmatrix} \tag{8}$$

with the matrix M taking the form,

$$M = e^{i\varphi(t)\lambda_7} e^{i\phi(t)\lambda_2} e^{i\theta(t)\lambda_5} \tag{9}$$

and explicitly rotation matrix M turns out to be,

$$\begin{pmatrix} \cos\theta\cos\phi & \sin\phi & \cos\phi\sin\theta \\ -\sin\theta\sin\varphi - \cos\theta\cos\varphi\sin\phi & \cos\phi\cos\varphi & \cos\theta\sin\varphi - \sin\theta\cos\varphi\sin\phi \\ -\sin\theta\cos\varphi + \cos\theta\sin\phi\sin\varphi & -\cos\phi\sin\varphi & \cos\theta\cos\varphi + \sin\theta\sin\phi\sin\varphi \end{pmatrix} \tag{10}$$

Generators for First Method

where

$$\lambda_7 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \tag{11}$$

$$\lambda_5 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \tag{12}$$

$$\lambda_2 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{13}$$

Second Diagonalisation Method

2. Diagonlisation by SO(3) Group Structure

For the same kind of problem of time-dependent 3 CHO Hassoul et. al. used SO(3) Lie group method for doing diagonalisation of the Hamiltonian

$$H_1(t) = \frac{1}{2}\sum_{i=1}^{3}[\frac{p_i^2}{m_i(t)} + C_i(t)x_i^2] + \frac{1}{2}[C_{12}(t)x_1x_2 + C_{13}(t)x_1x_3 + C_{23}(t)x_2x_3] \quad (14)$$

here $m_i(t)$, $C_i(t)$ (i=1, 2, 3), $C_{12}(t)$, $C_{13}(t)$, $C_{23}(t)$ are the arbitrary time-dependent model parameters.
Like Merdaci and Jellal's approach Eqn.(14) can be written in the matrix form

$$H_2(t) = \frac{1}{2}\sum_{i,j=1}^{3} P_i\delta_{ij}P_j + \frac{1}{2}\sum_{i,j=1}^{3} X_i\Gamma_{ij}(t)X_j \quad (15)$$

Second Diagonalisation Method

Where the model parameters matrix can be written as

$$\Gamma(t) = \begin{pmatrix} \bar{w_1}^2 & \frac{1}{2}K_{12}(t) & \frac{1}{2}K_{13}(t) \\ \frac{1}{2}K_{12}(t) & \bar{w_2}^2 & \frac{1}{2}K_{23}(t) \\ \frac{1}{2}K_{13}(t) & \frac{1}{2}K_{23}(t) & \bar{w_3}^2 \end{pmatrix} \tag{16}$$

here

$$\bar{w}_i^2(t) = \frac{C_i(t)}{m_i(t)} + \frac{1}{4}(\frac{\dot{m_i}^2(t)}{m_i^2(t)} - \frac{2\ddot{m}_i(t)}{m_i(t)}), \tag{17}$$

$$K_{12} = \frac{C_{12}(t)}{\sqrt{m_1(t)m_2(t)}}, \quad K_{13} = \frac{C_{13}(t)}{\sqrt{m_1(t)m_3(t)}}, \quad K_{23} = \frac{C_{23}(t)}{\sqrt{m_2(t)m_3(t)}} \tag{18}$$

Second Diagonalisation Method

The rotation matrix for diagonalisation of the Hamiltonian used is

$$\mathbb{R} = \mathbb{R}_{x_1}(\phi)\ \ \mathbb{R}_{x_2}(\theta)\ \ \mathbb{R}_{x_3}(\varphi) \tag{19}$$

here

$$\mathbb{R}_{x_1}(\phi) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\phi & -\sin\phi \\ 0 & \sin\phi & \cos\phi \end{pmatrix} \tag{20}$$

$$\mathbb{R}_{x_2}(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix} \tag{21}$$

$$\mathbb{R}_{x_3}(\varphi) = \begin{pmatrix} \cos\varphi & -\sin\varphi & 0 \\ \sin\varphi & \cos\varphi & 0 \\ 0 & 0 & 1 \end{pmatrix} \tag{22}$$

Second Diagonalisation Method

- This should be noted that the above rotation matrices are there when we move the frame anticlockwise and thus results in the following rotation matrix $\mathbb{R}$.
- Notice the difference in minus sign in some terms and column 2 and column 3 interchanged due to the change in the order of matrix multiplication with respect to Eqn.(10)

$$\begin{pmatrix} \cos\theta\cos\phi & -\cos\theta\sin\varphi & \sin\theta \\ \cos\phi\sin\varphi + \sin\phi\sin\theta\cos\varphi & \cos\phi\cos\varphi - \sin\phi\sin\theta\sin\varphi & -\sin\phi\cos\theta \\ \sin\phi\sin\varphi - \cos\phi\sin\theta\cos\varphi & \sin\phi\cos\varphi + \cos\phi\sin\theta\sin\varphi & \cos\phi\cos\theta \end{pmatrix} \tag{23}$$

This $\mathbb{R}$ matrix is now derived by using the generators of SO(3) Lie group as follows

$$\Lambda(t) = \mathbb{R} = \mathrm{e}^{\mathrm{i}\phi(\mathrm{t})\mathrm{J}_1}\mathrm{e}^{\mathrm{i}\theta(\mathrm{t})\mathrm{J}_2}\mathrm{e}^{\mathrm{i}\varphi(\mathrm{t})\mathrm{J}_3} \tag{24}$$

Generators for Second Method

where

$$J_1 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix} \tag{25}$$

$$J_2 = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix} \tag{26}$$

$$J_3 = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \tag{27}$$

Connection Between Two Methods of Diagonlisation

1. For establishing the connection of the two methods, we shall bring it out by first comparing the model parameter matrices from Merdaci and Jellal and Hassoul et. al. respectively

$$R(t) = \begin{pmatrix} w_1^2(t) & J_{12}(t) & J_{13}(t) \\ J_{12}(t) & w_2^2(t) & J_{23}(t) \\ J_{13}(t) & J_{23}(t) & w_3^2(t) \end{pmatrix}, \ \Gamma(t) = \begin{pmatrix} \bar{w_1}^2(t) & \frac{1}{2}K_{12}(t) & \frac{1}{2}K_{13}(t) \\ \frac{1}{2}K_{12}(t) & \bar{w_2}^2(t) & \frac{1}{2}K_{23}(t) \\ \frac{1}{2}K_{13}(t) & \frac{1}{2}K_{23}(t) & \bar{w_3}^2(t) \end{pmatrix}$$

These two matrices can be shown as equivalent.

Connection Between Two Methods of Diagonlisation

2. If we look carefully the transformation matrices of the two methods, we shall easily notice the similarity. Merdaci and Jellal used the following transformation matrix M for diagonalisation.

$$\begin{pmatrix} \cos\theta\cos\phi & \sin\phi & \cos\phi\sin\theta \\ -\sin\theta\sin\varphi - \cos\theta\cos\varphi\sin\phi & \cos\phi\cos\varphi & \cos\theta\sin\varphi - \sin\theta\cos\varphi\sin\phi \\ -\sin\theta\cos\varphi + \cos\theta\sin\phi\sin\varphi & -\cos\phi\sin\varphi & \cos\theta\cos\varphi + \sin\theta\sin\phi\sin\varphi \end{pmatrix}$$

whereas the Hassoul et. al. used the transformation matrix $\Lambda = \mathbb{R}$ as follows

$$\begin{pmatrix} \cos\theta\cos\phi & -\cos\theta\sin\varphi & \sin\theta \\ \cos\phi\sin\varphi + \sin\phi\sin\theta\cos\varphi & \cos\phi\cos\varphi - \sin\phi\sin\theta\sin\varphi & -\sin\phi\cos\theta \\ \sin\phi\sin\varphi - \cos\phi\sin\theta\cos\varphi & \sin\phi\cos\varphi + \cos\phi\sin\theta\sin\varphi & \cos\phi\cos\theta \end{pmatrix}$$

Connection Between Two Methods of Diagonlisation

3. Generators to construct M matrix by Merdaci and Jellal is

$$M = e^{i\varphi(t)\lambda_7} e^{i\phi(t)\lambda_2} e^{i\theta(t)\lambda_5}$$

Whereas for $\mathbb{R} = \Lambda$ matrix by Hassoul et. al. is

$$\Lambda = \mathbb{R} = \mathrm{e}^{\mathrm{i}\phi(\mathrm{t})\mathrm{J}_1} \mathrm{e}^{\mathrm{i}\theta(\mathrm{t})\mathrm{J}_2} \mathrm{e}^{\mathrm{i}\varphi(\mathrm{t})\mathrm{J}_3}$$

One can see the set of generators $(\lambda_7,\ \lambda_5,\ \lambda_2)$ is equivalent to $(J_1,\ J_2,\ J_3)$ respectively.

- This is the fundamental reason why the transformation matrix of the two diagonalisation methods is matching.
- Thus it is clear from the above discussion that the mathematical structures of the methods originate from the same basic formalism of matching generators of SU(3) and SO(3) Lie algebras.

Conditions for Existence of Bound States

- To make this analysis as broad as possible we shall consider the Hamiltonian operator as a quadratic function in terms of dynamical variables as follows

$$H(t) = \frac{1}{2}\left(p^t K p + x^t V x\right) \tag{29}$$

with $p^t = (p_1\ p_2\ ...\ p_M)$, $x_t = (x_1\ x_2\ ...\ x_M)$ (t designates transpose) and K, V represent $M \times M$ symmetric matrices with real entries.

- We know that the canonical transformation

$$x = \Lambda x', \quad \text{and} \quad p = (\Lambda)^{-1} p' \tag{30}$$

makes sure for transformed coordinates $x'^t = (x'_1\ x'_2\ ...\ x'_M)$ and momenta $p'^t = (p'_1\ p'_2\ ...\ p'_M)$ obeying $[x'_i,\ p'_j] = i\hbar\delta_{ij}$.

- We shall consider the $M \times M$ matrix Λ such that

$$\Lambda^{-1} K (\Lambda^t)^{-1} = I, \quad \Lambda^t V \Lambda = D \tag{31}$$

with I and D being the $M \times M$ identity and diagonal matrix respectively. The matrix D has elements e_i, $i = 1, 2, ...M$.

- Thus, the Hamiltonian (29) reduces to

$$H(t) = \frac{1}{2}(p'^{t} p' + x^{t'} D x') \tag{32}$$

Obviously, we shall have bound states if $e_i > 0, i = 1, 2, ..., M$.

- Due to the commutation relations between transformed coordinates and momenta, the eigenvalues are as follows

$$E_m = \hbar \sum_{i=1}^{M} \sqrt{e_i} \left(m_i + \frac{1}{2} \right), m = m_1, m_2, ..., m_M, m_i = 0, 1, 2, ... \tag{33}$$

- Eqn.(31) can give us

$$\Lambda^{-1} K V \Lambda = D \tag{34}$$

such that the complete problem boils down to the diagonalisation for the non-symmetric matrix $B = KV$.

Conditions for Existence of Bound States

- Eqn.(34) can be written as follows

$$U^{-1}K^{\frac{1}{2}}VK^{\frac{1}{2}}U = D \tag{35}$$

  which is possible only if the matrix K is positive definite that allows one to write $\Lambda = K^{\frac{1}{2}}U$.
- Due to $T = K^{\frac{1}{2}}VK^{\frac{1}{2}}$ being symmetric, U becomes orthogonal and one can employ familiar systematic diagonalisation methods.
- The symmetric matrix T turns out to be more appropriate for finding model parameters which are consistent with positive eigenvalues e_i and, hence, bound states. It is a familiar theorem that if every leading minor of a symmetric matrix is positive then only a symmetric matrix is positive definite.
- We shall demonstrate it by an example.

Bound State Conditions for Model by Hassoul et. al.

The example we take up was Hamiltonian H(t) studied by Hassoul et. al.

$$\frac{1}{2}\sum_{i=1}^{3}\left[\frac{P_i^2}{m_i(t)}+C_i(t)X_i^2\right]+\frac{1}{2}\left[C_{12}(t)X_1X_2+C_{13}(t)X_1X_3+C_{23}(t)X_2X_3\right] \tag{36}$$

is a special case of the general model (29) with $M=3$ and a positive-definite diagonal matrix K with entries $K_{ij}=\delta_{ij}/m_i(t)$. The pertinent matrices for the diagonalisation of (36) are

$$B(t)=KV=\begin{pmatrix} w_1^2(t) & \frac{C_{12}(t)}{2m_1(t)} & \frac{C_{13}(t)}{2m_1(t)} \\ \frac{C_{12}(t)}{2m_2(t)} & w_2^2(t) & \frac{C_{23}(t)}{2m_2(t)} \\ \frac{C_{13}(t)}{2m_3(t)} & \frac{C_{23}(t)}{2m_3(t)} & w_3^2(t) \end{pmatrix} \tag{37}$$

Bound State Conditions for Model by Hassoul et. al.

$$T(t) = \begin{pmatrix} w_1^2(t) & \frac{C_{12}(t)}{2\sqrt{m_1(t)m_2(t)}} & \frac{C_{13}(t)}{2\sqrt{m_1(t)m_3(t)}} \\ \frac{C_{12}(t)}{2\sqrt{m_1(t)m_2(t)}} & w_2^2(t) & \frac{C_{23}(t)}{2\sqrt{m_2(t)m_3(t)}} \\ \frac{C_{13}(t)}{2\sqrt{m_1(t)m_3(t)}} & \frac{C_{23}(t)}{2\sqrt{m_2(t)m_3(t)}} & w_3^2(t) \end{pmatrix} \quad (38)$$

where the matrix $\Gamma(t)$ in Hassoul et. al. is identical to T(t). Thus, the orthogonal U matrix shown above should be equal to $\mathbb{R} = \Lambda$ matrix in Hassoul et. al

Bound State Conditions for Model by Hassoul et. al.

- Any of those matrices (with the multiplication of -1) have the following characteristic polynomial

$$\xi^3 - d\xi^2 + e\xi - f = 0, \text{ with } d = w_1^2(t) + w_2^2(t) + w_3^2(t).$$

Likewise we have expressions for e and f. The three non-zero roots of the polynomial are the diagonal entries of the diagonal matrix D.

- When the 3 roots turn out to be real and positive, then $d > 0$ and $f > 0$.
- Such constraints are necessary but not sufficient due to being consistent with two complex-conjugate roots having a real part positive and one root which is positive.
- To avoid the former condition we include the characteristic polynomial determinant as follows

$$\Delta = (\xi_1-\xi_2)^2(\xi_1-\xi_3)^2(\xi_2-\xi_3)^2 = d^2e^2-4d^3f+18def-4e^3-27c^2 \geq 0 \quad (39)$$

Necessary and Sufficient Conditions

- We can now derive without much difficulty amazingly simple necessary and sufficient constraints that ensure the existence of bound state solutions of three time-dependent CQHO by using T matrix's principle minors as follows

1.

$w_1^2 > 0$

2.

$4m_1(t)m_2(t)w_1^2(t)w_2^2(t) - C_{12}^2(t) > 0$

3.

$$4m_1(t)m_2(t)m_3(t)w_1^2(t)w_2^2(t)w_3^2(t) + C_{12}(t)C_{13}(t)C_{23}(t)$$
$$-m_1(t)w_1^2(t)C_{23}^2(t) - m_2(t)w_2^2(t)C_{13}^2(t) - m_3(t)w_3^2(t)C_{12}^2(t) > 0$$

Conclusions and Future Outlook

1.

We have established the diagonalisation methods which look quite different for solving 3 coupled harmonic oscillators used in Merdaci and Jellal and Hassoul et. al. are fundamentally the same in mathematical sense.

2.

In Merdaci and Jellal, their transformation matrix has been shown to be equivalent to one used by Hassoul et. al. when the matching was done at the level of generators one by one.

3.

This also clears some of the issues reported recently by Rahma et. al.

4.

Then we established necessary and sufficient conditions for time-dependent 3 CQHO that is valid for the time-independent case as well.

Conclusions and Future Outlook

5.

Our analysis has revealed the model parameter values for time-dependent 3 CQHO that are compatible with the bound states which were not analyzed earlier in the literature to the best of our knowledge.

6.

Besides revealing the necessary and sufficient conditions regarding time-dependent 3 CQHO, our work also brings into focus a familiar method for considering more general configurations of coupled harmonic oscillators.

7.

After solving CQHO, one can start a quantum simulation of such systems.

8.

The first step towards it will be to write down a quantum algorithm analytically. Such directions are under considerations at the moment.

Thank You