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Application of the 'invariant eigen-operator' and energy-level gap

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Abstract: *We apply the conception of 'invariant eigen-operator' of the square of the Schrödinger operator which is proposed by H. Y. Fan and C. Li to some molecule oscillator models and we find more 'invariant eigen-operators'.*
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I. Introduction

H. Y. Fan and C. Li [1] suggest that the invariant eigen-operator $\hat{O}_e$ satisfies

$$\left(i\frac{d}{dt}\right)^2 \hat{O}_e = \left[\left[\hat{O}_e, \hat{H}\right], \hat{H}\right] = \lambda \hat{O}_e , \tag{1}$$

noticing from the Heisenberg equation

$$i\frac{d}{dt}\,\hat{O}_e = \frac{1}{i}\left[\hat{O}_e, \hat{H}\,\right] \qquad \text{for } \hbar = 1.$$

And they judge that $\sqrt{\lambda}$ in (1) is the energy gap between two adjacent eigenstates of the Hamiltonian $\hat{H}$.

In this article we use the conception of 'invariant eigen-operator' so that we can obtain the energy gap in two-mode coupled oscillators and find more another 'invariant eigen-operators' in bi-atomic and triatomic molecule systems.

II. Some results

The model of two coupled time-dependent harmonic oscillators has been studied by many authors and applied to describe quantum amplifiers and converters. The Hamiltonian [2] for the model is

$$H = \omega_a\, a^\dagger a + \omega_b\, b^\dagger b + g(a^\dagger b + b^\dagger a) , \tag{2}$$

where a (b) and $a^\dagger$ $(b^\dagger)$ are annihilation and creation operators for each of one of the interacting modes of frequency ω_a and ω_b, obeying $[a^\dagger, a] = -1$ $([b^\dagger, b] = -1)$ and $g(> 0)$ is the coupling constant.

Theorem 2.1. For the two-mode coupled oscillators, the energy gap between two states is

$$\Delta E = \sqrt{{\omega_a}^2 + l\, g(\omega_a + \omega_b) + g^2} ,$$

where the coefficient l is given by

$$l = \frac{\omega_b - \omega_a \pm \sqrt{(\omega_b - \omega_a)^2 + 4g^2}}{2g} .$$

Proof. By using Eq. (2) and the Heisenberg equation of motion, we have

$$\begin{aligned} i\frac{d}{dt}a &= [a, H] = [a, \omega_a a^\dagger a + \omega_b\, b^\dagger b + g(a^\dagger b + b^\dagger a)] \\ &= \omega_a [a, a^\dagger a] + \omega_b [a, b^\dagger b] + g([a, a^\dagger b] + [a, b^\dagger a]) \\ &= \omega_a (a^\dagger [a, a] + [a, a^\dagger] a) + \omega_b (b^\dagger [a, b] + [a, b^\dagger] b) \\ &\quad + g(a^\dagger [a, b] + [a, a^\dagger] b + b^\dagger [a, a] + [a, b^\dagger] a) \\ &= \omega_a a + g b . \end{aligned} \tag{3}$$

Similarly, we obtain

$$i\frac{d}{dt}b = [b,H] = \omega_b b + ga . \tag{4}$$

To find one of the 'invariant eigen-operators' of $\left(i\frac{d}{dt}\right)^2$ we put $\hat{O}_e = a + lb$. Then by (1), (3), and (4), we observe that

$$\begin{aligned}(\Delta E)^2(a+lb) &= (\Delta E)^2\hat{O}_e \\ &= \left(i\frac{d}{dt}\right)^2\hat{O}_e \\ &= \left[\left[\hat{O}_e,\hat{H}\right],\hat{H}\right] \\ &= \left[\left[a+lb,\hat{H}\right],\hat{H}\right] \\ &= \left[\left[a,\hat{H}\right]+l\left[b,\hat{H}\right],\hat{H}\right] \\ &= \left[\omega_a a + gb + l(\omega_b b + ga),\hat{H}\right] \\ &= (\omega_a + lg)\left[a,\hat{H}\right] + (g + l\omega_b)\left[b,\hat{H}\right] \\ &= (\omega_a+lg)(\omega_a a + gb) + (g+l\omega_b)(\omega_b b + ga) \\ &= \{{\omega_a}^2 + lg(\omega_a+\omega_b) + g^2\}a + l\left\{\frac{g}{l}(\omega_a+\omega_b) + g^2 + {\omega_b}^2\right\}b\end{aligned} \tag{5}$$

and so we claim that

$${\omega_a}^2 + gl(\omega_a+\omega_b) + g^2 = \frac{g}{l}(\omega_a+\omega_b) + g^2 + {\omega_b}^2 .$$

Solving this we have

$$l({\omega_a}^2 - {\omega_b}^2) + gl^2(\omega_a+\omega_b) - g(\omega_a+\omega_b) = 0$$

and

$$(\omega_a+\omega_b)g\left(l^2 + \frac{\omega_a-\omega_b}{g}l - 1\right) = 0,$$

which implies that

$$l = \frac{-\frac{\omega_a-\omega_b}{g} \pm \sqrt{\left(\frac{\omega_a-\omega_b}{g}\right)^2+4}}{2} = \frac{\omega_b-\omega_a \pm \sqrt{(\omega_b-\omega_a)^2+4g^2}}{2g} .$$

Adopting this l, we can rewrite Eq. (5) as

$$(\Delta E)^2\hat{O}_e = \{{\omega_a}^2 + lg(\omega_a+\omega_b) + g^2\}\hat{O}_e ,$$

therefore, the proof is complete. □

Example 2.2. Let us consider the special case $\omega_a = \omega_b\ (:= \omega)$ of Theorem 2.1. Then $l = \pm 1$ and the energy-level gap

$$\Delta E = \sqrt{\omega^2 \pm 2\,g\omega + g^2} = \omega \pm g ,$$

which coincides with [1].

The Hamiltonian that describes bi-atomic molecule is [1, 3]

(6) $$H = \frac{1}{2m}\,(P_1^2 + P_2^2) + \frac{1}{2}\,m\omega^2(x_1^2 + x_2^2) - \lambda\, x_1 x_2$$

and it satisfies the following commutation relations:

(7) $$[x_1, H] = \frac{iP_1}{m}\,, \qquad [P_1, H] = -im\omega^2 x_1 + i\lambda x_2\,,$$
$$[x_2, H] = \frac{iP_2}{m}\,, \qquad [P_2, H] = -im\omega^2 x_2 + i\lambda x_1\,.$$

H. Y. Fan and C. Li suppose

(8) $$\hat{O}_{1e} = x_1 \pm x_2$$

as the 'invariant eigen-operator' of (6) to obtain the energy-level gap

(9) $$\Delta E = \sqrt{\left(\omega^2 \mp \frac{\lambda}{m}\right)}\,,$$

respectively, in [1]. We find another 'invariant eigen-operator' of (6) to get the same energy-level gap in the below corollary.

Corollary 2.3. One of the 'invariant eigen-operators' of bi-atomic molecule model is

$$\hat{O}_{2e} = P_1 \pm P_2\,.$$

Proof. By using the given 'invariant eigen-operator', (1), and (7), we deduce that

$$\begin{aligned}
(\Delta E)^2 \hat{O}_{2e} &= \left(i\frac{d}{dt}\right)^2 \hat{O}_{2e} \\
&= \left[\left[\hat{O}_{2e}, \hat{H}\right], \hat{H}\right] \\
&= \left[\left[P_1 \pm P_2, \hat{H}\right], \hat{H}\right] \\
&= i(-m\omega^2 \pm \lambda)[x_1, H] + i\,(\lambda \mp m\omega^2)\,[x_2, H] \\
&= i(-m\omega^2 \pm \lambda)\cdot\frac{iP_1}{m} + i\,(\lambda \mp m\omega^2)\cdot\frac{iP_2}{m} \\
&= \left(\omega^2 \mp \frac{\lambda}{m}\right)P_1 \pm \left(\omega^2 \mp \frac{\lambda}{m}\right)P_2 \\
&= \left(\omega^2 \mp \frac{\lambda}{m}\right)(P_1 \pm P_2) \\
&= \left(\omega^2 \mp \frac{\lambda}{m}\right)\hat{O}_{2e}
\end{aligned}$$

and so it coincides with (9). □

Remark 2.4. Let $\hat{O}_{3e} = \hat{O}_{1e} + \hat{O}_{2e}$. Then from (8), (9), and Corollary 2.3 we lead that

$$\begin{aligned}
(\Delta E)^2 \hat{O}_{3e} &= (\Delta E)^2 (x_1 \pm x_2 + P_1 \pm P_2) \\
&= \left(\omega^2 \mp \frac{\lambda}{m}\right)(x_1 \pm x_2 + P_1 \pm P_2) \\
&= \left(\omega^2 \mp \frac{\lambda}{m}\right)\hat{O}_{3e}
\end{aligned}$$

and so we discover another 'invariant eigen-operator' of (6) is $\hat{O}_{3e} = x_1 \pm x_2 + P_1 \pm P_2$. This fact arouses the idea of Lemma 2.5.

Lemma 2.5. Let V and W be the sets of 'invariant eigen-operators' with the same energy-level gap. Then the mapping

$$\left(i\frac{d}{dt}\right)^2 : V \rightarrow W$$

is a linear map.

Proof. Let $\hat{O}_{1e}, \hat{O}_{2e} \in V$ with the same energy-level gap ΔE, i.e., by (1) we have

$$\left(i\frac{d}{dt}\right)^2 \hat{O}_{1e} = \left[\left[\hat{O}_{1e}, \hat{H}\right], \hat{H}\right] = (\Delta E)^2 \hat{O}_{1e}$$

and

$$\left(i\frac{d}{dt}\right)^2 \hat{O}_{2e} = \left[\left[\hat{O}_{2e}, \hat{H}\right], \hat{H}\right] = (\Delta E)^2 \hat{O}_{2e} .$$

Thus, we can show that

$$\begin{aligned} \left(i\frac{d}{dt}\right)^2 \hat{O}_{1e} + \left(i\frac{d}{dt}\right)^2 \hat{O}_{2e} &= (\Delta E)^2 \hat{O}_{1e} + (\Delta E)^2 \hat{O}_{2e} \\ &= (\Delta E)^2 \left(\hat{O}_{1e} + \hat{O}_{2e}\right) \\ &= \left(i\frac{d}{dt}\right)^2 \left(\hat{O}_{1e} + \hat{O}_{2e}\right) . \end{aligned}$$

Moreover, for any constant $\alpha \in \mathbb{C}$ we obtain

$$\begin{aligned} \left(i\frac{d}{dt}\right)^2 \left(\alpha \hat{O}_{1e}\right) &= \left[\left[\alpha \hat{O}_{1e}, \hat{H}\right], \hat{H}\right] \\ &= \left[\alpha\left[\hat{O}_{1e}, \hat{H}\right], \hat{H}\right] \\ &= \alpha\left[\left[\hat{O}_{1e}, \hat{H}\right], \hat{H}\right] \\ &= \alpha\left(i\frac{d}{dt}\right)^2 \hat{O}_{1e} . \end{aligned}$$

□

The Hamiltonian operator that describes a linear triatomic molecule is [1, 4]

$$H = \frac{P_1^2}{2m} + \frac{P_2^2}{2M} + \frac{P_3^2}{2m} + \frac{\tau}{2}(x_2 - x_1 - \beta)^2 + \frac{\tau}{2}(x_3 - x_2 - \beta)^2 \tag{10}$$

and it signifies as follows:

$$\begin{aligned} [x_1, H] &= \frac{iP_1}{m}, & [P_1, H] &= i\tau(x_2 - x_1 - \beta), \\ [x_2, H] &= \frac{iP_2}{M}, & [P_2, H] &= i\tau(x_3 - 2x_2 + x_1), \\ [x_3, H] &= \frac{iP_3}{m}, & [P_3, H] &= i\tau(x_2 - x_3 + \beta). \end{aligned} \tag{11}$$

Similarly, in [1] H. Y. Fan and C. Li suggest

$$\hat{O}_{4e} = x_1 - x_3, \qquad \hat{O}_{5e} = x_1 - 2x_2 + x_3, \qquad \hat{O}_{6e} = x_1 + \frac{M}{m}x_2 + x_3 \tag{12}$$

as the 'invariant eigen-operator' of (10) to obtain the energy-level gap

(13) $$\Delta E = \sqrt{\frac{\tau}{m}}\,, \qquad \Delta E = \sqrt{\frac{\tau}{m}\left(1+\frac{2m}{M}\right)}\,, \qquad \Delta E = 0\,,$$

respectively. Thus, we find another 'invariant eigen-operator' of (10) to get the same energy-level gap in Theorem 2.6.

Theorem 2.6. In a linear triatomic molecule model, three of the 'invariant eigen-operators' are

$$\hat{O}_{1e} = P_1 - P_3\,,$$
$$\hat{O}_{2e} = P_1 - \frac{2m}{M}P_2 + P_3\,,$$
$$\hat{O}_{3e} = P_1 + P_2 + P_3$$

and their corresponding energy gap is

$$\Delta E_{1e} = \sqrt{\frac{\tau}{m}}\,,$$
$$\Delta E_{2e} = \sqrt{\frac{\tau}{m}\left(1+\frac{2m}{M}\right)}\,,$$
$$\Delta E_{3e} = 0\,.$$

Proof. For $l_2,\ l_3 \in \mathbb{R}$, we set

(14) $$\hat{O}_e = P_1 + l_2P_2 + l_3P_3\,.$$

Then by (1) and (11), we note that

(15)
$$\begin{aligned}
(\Delta E)^2\,(P_1 + l_2P_2 + l_3P_3) &= \left(i\frac{d}{dt}\right)^2 \hat{O}_e \\
&= \left[[\hat{O}_e,\hat{H}],\hat{H}\right] \\
&= \left[[P_1,\hat{H}] + l_2[P_2,\hat{H}] + l_3[P_3,\hat{H}],\hat{H}\right] \\
&= \left[i\tau(x_2 - x_1 - \beta) + l_2\cdot i\tau(x_3 - 2x_2 + x_1) + l_3\cdot i\tau(x_2 - x_3 + \beta),\hat{H}\right] \\
&= i\tau(-1 + l_2)[x_1,\hat{H}] + i\tau(1 - 2l_2 + l_3)[x_2,\hat{H}] + i\tau(l_2 - l_3)[x_3,\hat{H}] \\
&= i\tau(-1 + l_2)\cdot\frac{iP_1}{m} + i\tau(1 - 2l_2 + l_3)\cdot\frac{iP_2}{M} + i\tau(l_2 - l_3)\cdot\frac{iP_3}{m} \\
&= \frac{\tau(1-l_2)}{m}\left(P_1 - \frac{m(l_3 - 2l_2 + 1)}{M(1-l_2)}P_2 + \frac{l_3 - l_2}{1-l_2}P_3\right)
\end{aligned}$$

and

(16) $$\Delta E = \sqrt{\frac{\tau(1-l_2)}{m}}\,, \qquad l_2 = -\frac{m(l_3 - 2l_2 + 1)}{M(1-l_2)}\,, \qquad l_3 = \frac{l_3 - l_2}{1-l_2}$$

for $l_2 \neq 1$. The 3rd identity of (16) shows that

$$l_3(1-l_2) = l_3 - l_2 \quad\Rightarrow\quad l_2(l_3 - 1) = 0 \quad\Rightarrow\quad l_2 = 0 \ \text{ or } \ l_3 = 1\,.$$

Case 1] Where $l_2 = 0$; By (14) and (16) we have

$$\frac{m(l_3+1)}{M} = 0 \qquad\Rightarrow\qquad l_3 = -1$$

and so

$$\Delta E_{1e} = \sqrt{\frac{\tau}{m}}, \qquad \hat{O}_{1e} = P_1 - P_3 .$$

Case 2] Where $l_3 = 1$; From (14) and (16) we obtain

$$\begin{aligned} l_2 = -\frac{m(2-2l_2)}{M(1-l_2)} \quad &\Rightarrow \quad l_2 M(1-l_2) = 2m(l_2 - 1) \\ &\Rightarrow \quad M l_2^2 + (2m - M) l_2 - 2m = 0 \\ &\Rightarrow \quad (M l_2 + 2m)(l_2 - 1) = 0 \\ &\Rightarrow \quad l_2 = 1 \quad \text{or} \quad l_2 = -\frac{2m}{M} \\ &\Rightarrow \quad l_2 = -\frac{2m}{M}, \end{aligned}$$

since $l_2 = 1$ contradicts to the condition $l_2 \neq 1$. Thus

$$\Delta E_{2e} = \sqrt{\frac{\tau}{m}\left(1 + \frac{2m}{M}\right)}, \qquad \hat{O}_{2e} = P_1 - \frac{2m}{M} P_2 + P_3 .$$

Case 3] Where $l_2 = 1$; By (14) and (15) we observe that

$$(\Delta E)^2 (P_1 + P_2 + l_3 P_3) = \tau(1 - l_3)\left(\frac{P_2}{M} - \frac{P_3}{m}\right)$$

and so

$$\Delta E_{3e} = 0, \qquad l_3 = 1$$

therefore, we conclude that

$$\hat{O}_{3e} = P_1 + P_2 + P_3 .$$

□

Finally, as an application of Lemma 2.5 we consider (12), (13), and Theorem 2.6. Then another three of the 'invariant eigen-operator' on the Eq. (10) are

$$\begin{aligned} \hat{O}_{7e} &= x_1 - x_3 + P_1 - P_3 , \\ \hat{O}_{8e} &= x_1 - 2x_2 + x_3 + P_1 - \frac{2m}{M} P_2 + P_3 , \\ \hat{O}_{9e} &= x_1 + \frac{M}{m} x_2 + x_3 + P_1 + P_2 + P_3 . \end{aligned}$$

III. Conclusion

In the harmonic oscillator models, we consider the energy-level gap and deduce the new 'invariant eigen-operators' from the existing eigen-operators.

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