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Squeezing in the triatomic linear molecule model revealed by virtue of the IWOP technique

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Abstract. For a typical triatomic linear molecule with different atomic masses we find a unitary operator which is closely related to squeezing transformations caused by frequency jumps. The coordinate representation of the unitary operator is identified, which provides an alternative approach for calculating the wavefunction of the internal motion of the molecule. We also show that the unitary operator is equivalent to a two-mode squeezing-rotating combination operator multiplied from the right by two single-mode squeezing operators. Our discussion is mainly based on the technique of integration within an ordered product (IWOP) of operators.

1. Introduction

Recently much attention has been paid to squeezed states of photons and harmonic oscillators [1, 2]. Formally, these states are generated from coherent states by appropriate squeeze operators. An approach for obtaining the normally ordered form of squeeze operators, which uses the technique of integration within an ordered product (IWOP) of operators, is presented in [3, 4]. An explicit interpretation of the squeezing as a symplectic transformation in coordinate or momentum variables is an interesting result of this approach. The general symplectic transformation for SP(4) has been studied by Moshinsky [5] and the fact that the two-mode squeezing operator belongs to the SP(4) generators pointed out by Milburn [6]. In this work we show that squeezing mechanism exists in solving the wavefunction of a triatomic linear molecule. A well defined unitary operator U, which includes both squeezing and rotating transformations and can directly lead us to obtain the wavefunction, can be found in terms of the IWOP technique. Let us briefly review the way of dealing with the molecule's dynamics in [7] where bending vibrations are not taken into account. The Hamiltonian is given by

$$H=-\frac{\hbar^2}{2}\sum_{i=1}^{3}\frac{1}{m_i}\frac{\partial^2}{\partial x_i^2}+\frac{k}{2}[(x_2-x_1-d)^2+(x_3-x_2-d)^2] \tag{1}$$

where d is the distance between two adjacent atoms. Using the coordinates transformation

$$\xi=(x_2-x_1)-d \qquad \eta=(x_3-x_2)-d \tag{2a}$$

$$X=\frac{1}{M}(m_1x_2+m_2x_2+m_3x_3) \qquad M=m_1+m_2+m_3 \tag{2b}$$

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and consequently,

$$\frac{\partial}{\partial x_1}=\frac{m_1}{M}\frac{\partial}{\partial X}-\frac{\partial}{\partial \xi} \qquad \frac{\partial}{\partial x_2}=\frac{m_2}{M}\frac{\partial}{\partial X}+\frac{\partial}{\partial \xi}-\frac{\partial}{\partial \eta} \qquad \frac{\partial}{\partial x_3}=\frac{m_3}{M}\frac{\partial}{\partial X}+\frac{\partial}{\partial \eta}. \tag{3}$$

The Hamiltonian is put into the separable form $H=H_{CM}+H_i$, where

$$H_{CM}=\frac{P_M^2}{2M} \qquad P_M=-i\hbar\frac{\partial}{\partial X}$$

$$H_i=-\frac{\hbar^2}{2\mu_1}\frac{\partial^2}{\partial \xi^2}-\frac{\hbar^2}{2\mu_2}\frac{\partial^2}{\partial \eta^2}+\frac{\hbar^2}{m_2}\frac{\partial^2}{\partial \xi\partial \eta}+\frac{k}{2}(\xi^2+\eta^2) \tag{4}$$

$$\mu_1\equiv\frac{m_1m_2}{m_1+m_2} \qquad \mu_2\equiv\frac{m_2m_3}{m_2+m_3}.$$

The motion of the centre-of-mass is thus separated off. Writing

$$-i\hbar\frac{\partial}{\partial \xi}=P_\xi \qquad -i\hbar\frac{\partial}{\partial \eta}=P_\eta$$

so $[\eta, P_\eta]=[\xi, P_\xi]=i\hbar$, and introducing the two-mode annihilation operators (a_ξ, a_η) by

$$\begin{aligned} a_\xi&=\frac{1}{\sqrt{2}}\left[\left(\frac{k\mu_1}{\hbar^2}\right)^{1/4}\xi+i\frac{P_\xi}{(k\mu_1\hbar^2)^{1/4}}\right] \\ a_\eta&=\frac{1}{\sqrt{2}}\left[\left(\frac{k\mu_2}{\hbar^2}\right)^{1/4}\eta+i\frac{P_\eta}{(k\mu_2\hbar^2)^{1/4}}\right] \end{aligned} \tag{5}$$

we can express H_i as (let $\omega_1=\sqrt{k/\mu_1}$, $\omega_2=\sqrt{k/\mu_2}$)

$$\begin{aligned} H_i&=\frac{1}{2\mu_1}P_\xi^2+\frac{1}{2\mu_2}P_\eta^2+\frac{k}{2}(\xi^2+\eta^2)-\frac{1}{m_2}P_\xi P_\eta \\ &=\omega_1\hbar\left(a_\xi^\dagger a_\xi+\frac{1}{2}\right)+\omega_2\hbar(a_\eta^\dagger a_\eta+\tfrac{1}{2})-\frac{1}{m_2}P_\xi P_\eta. \end{aligned} \tag{6}$$

After performing the rotation [7]

$$\xi'=\xi\cos\alpha+\eta\sin\alpha \qquad \eta'=-\xi\sin\alpha+\eta\cos\alpha \tag{7}$$

where α satisfies the condition

$$(m_3^{-1}-m_1^{-1})\sin 2\alpha=2m_2^{-1}\cos 2\alpha. \tag{8}$$

H_i is diagonalized as

$$\begin{aligned} H_i&=-\frac{\hbar^2}{2}\left(\frac{1}{A}\frac{\partial^2}{\partial \xi'^2}+\frac{1}{B}\frac{\partial^2}{\partial \eta'^2}\right)+\frac{k}{2}(\xi'^2+\eta'^2) \\ &\equiv\frac{1}{2A}P_{\xi'}^2+\frac{1}{2B}P_{\eta'}^2+\frac{k}{2}(\xi'^2+\eta'^2) \end{aligned}$$

where

$$\begin{aligned} A^{-1}&=\mu_1^{-1}\cos^2\alpha+\mu_2^{-1}\sin^2\alpha-m_2^{-1}\sin 2\alpha \\ B^{-1}&=\mu_1^{-1}\sin^2\alpha+\mu_2^{-1}\cos^2\alpha+m_2^{-1}\sin 2\alpha. \end{aligned} \tag{9}$$

By introducing the corresponding creation and annihilation operators

$$a_{\xi'}=\frac{1}{\sqrt{2}}\left[\left(\frac{kA}{\hbar^2}\right)^{1/4}\xi'+\mathrm{i}\frac{P_{\xi'}}{(kA\hbar^2)^{1/4}}\right]$$
$$a_{\eta'}=\frac{1}{\sqrt{2}}\left[\left(\frac{Bk}{\hbar^2}\right)^{1/4}\eta'+\frac{\mathrm{i}P_{\eta'}}{(Bk\hbar^2)^{1/4}}\right] \tag{10}$$

we rewrite H_i as

$$H_1=\omega_A\hbar(a^\dagger_{\xi'}a_{\xi'}+\tfrac{1}{2})+\omega_B\hbar(a^\dagger_{\eta'}a_{\eta'}+\tfrac{1}{2}) \qquad (\omega_A=\sqrt{k/A},\ \omega_B=\sqrt{k/B}) \tag{11}$$

whose eigenvector is $|n_1, n_2\rangle'=(n_1!n_2!)^{-1/2}a^{\dagger n_1}_{\xi'}a^{\dagger n_2}_{\eta'}|00\rangle'$, where $|00\rangle'$ is annihilated by $a_{\xi'}$ and $a_{\eta'}$. Based on the above review, in section 2 we identify U with a (ξ, η) coordinate representation, and then decompose U as a product of a two-mode rotating-squeezing combination operator and two single-mode squeezing operators. They can both be put into normally ordered forms by virtue of the IWOP technique. With these forms in hand, in section 3 we prove the correctness of the identification of U, which means that U can transform the eigenstate $|n_1n_2\rangle$ of $a^\dagger_\xi a_\xi+a^\dagger_\eta a_\eta$ to $|n_1, n_2\rangle'$, and includes both squeezing and rotating transformation. In section 4 we show that U's coordinate representation conveniently leads us to derive the wavefunction of the molecule.

2. The identification and analysis of U

We begin by postulating the following (ξ, η) coordinate representation of the required operator U

$$U=\left(\frac{\mu_1\mu_2}{AB}\right)^{1/8}\iint_{-\infty}^{\infty}\mathrm{d}\xi\,\mathrm{d}\eta\left|u\begin{pmatrix}\xi\\ \eta\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}\xi\\ \eta\end{pmatrix}\right| \qquad \left|\begin{pmatrix}\xi\\ \eta\end{pmatrix}\right\rangle\equiv|\xi\rangle|\eta\rangle=|\xi,\eta\rangle$$
$$u=\begin{pmatrix}(\mu_1/A)^{1/4}\cos\alpha & -(\mu_2/B)^{1/4}\sin\alpha\\ (\mu_1/A)^{1/4}\sin\alpha & (\mu_2/B)^{1/4}\cos\alpha\end{pmatrix} \qquad \det u=\left(\frac{\mu_1\mu_2}{AB}\right)^{1/4} \tag{12}$$

where the factor $(\mu_1\mu_2/AB)^{1/4}$ anticipates the normalization required to make U unitary, as will be seen later, and $|\xi, \eta\rangle$ is the coordinate eigenstate which in the Fock space spanned by $|n_1, n_2\rangle$ is given by

$$|\xi\rangle=\left(\frac{\mu_1\omega_1}{\pi\hbar}\right)^{1/4}\exp\left[-\frac{\mu_1\omega_1}{2\hbar}\xi^2+\sqrt{\frac{2\mu_1\omega_1}{\hbar}}\,\xi a^\dagger_\xi-\frac{1}{2}a^{\dagger 2}_\xi\right]|0\rangle_\xi\equiv|\xi\rangle_{\mu_1\omega_1} \tag{13}$$

$$|\eta\rangle=\left(\frac{\mu_2\omega_2}{\pi\hbar}\right)^{1/4}\exp\left[-\frac{\mu_2\omega_2}{2\hbar}\eta^2+\sqrt{\frac{2\mu_2\omega_2}{\hbar}}\,\eta a^\dagger_\eta-\frac{1}{2}a^{\dagger 2}_\eta\right]|0\rangle_\eta\equiv|\eta\rangle_{\mu_2\omega_2}. \tag{14}$$

The subscript $\mu_i\omega_i$ ($\mathrm{i}=1,2$) is to emphasize the $\mu_i\omega_i$ dependence of the state vectors. To check whether U is unitary, using (12) we calculate

$$UU^\dagger=\left(\frac{\mu_1\mu_2}{AB}\right)^{1/4}\iint_{-\infty}^{\infty}\mathrm{d}\xi\,\mathrm{d}\eta\left|u\begin{pmatrix}\xi\\ \eta\end{pmatrix}\right\rangle\left\langle u\begin{pmatrix}\xi\\ \eta\end{pmatrix}\right|$$
$$=\int_{-\infty}^{\infty}\mathrm{d}\eta|\xi\rangle\langle\xi|\int_{-\infty}^{\infty}\mathrm{d}\eta|\eta\rangle\langle\eta|=1 \tag{15}$$

because the Jacobian for the transformation of integration variables is just $(\mu_1\mu_2/AB)^{1/4}$. In terms of the normal product form of the vacuum projection operator

$$|00\rangle\langle 00|\equiv|0\rangle_\xi|0\rangle_\eta\,{}_\eta\langle 0|_\xi\langle 0|=\,:\exp[-a^\dagger_\xi a_\xi-a^\dagger_\eta a_\eta]: \tag{16}$$

where : : denotes the normal ordering, and with IWOP one is able to directly perform the integration in (12). However, a quite lengthy calculation would be needed. To avoid this and to analyse the U transformation more physically and clearly, according to the matrix decomposition of u

$$u = vs \qquad v \equiv \begin{pmatrix} \cos\alpha & -\sin\alpha \\ \sin\alpha & \cos\alpha \end{pmatrix} \qquad s \equiv \begin{pmatrix} (\mu_1/A)^{1/4} & 0 \\ 0 & (\mu_2/B)^{1/4} \end{pmatrix} \tag{17}$$

we decompose U as

$$\begin{gathered} U = VS_1S_2 \qquad V = \iint_{-\infty}^{\infty} \mathrm{d}\xi\,\mathrm{d}\eta \left| v\begin{pmatrix}\xi\\ \eta\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}\xi\\ \eta\end{pmatrix}\right| \\ S_1 = \left(\frac{\mu_1}{A}\right)^{1/8}\int_{-\infty}^{\infty}\mathrm{d}\xi\left|\left(\frac{\mu_1}{A}\right)^{1/4}\xi\right\rangle\langle\xi| \qquad S_2 = \left(\frac{\mu_2}{B}\right)^{1/8}\int_{-\infty}^{\infty}\mathrm{d}\eta\left|\left(\frac{\mu_2}{B}\right)^{1/4}\eta\right\rangle\langle\eta|. \end{gathered} \tag{18}$$

Here V is a two-mode rotating-squeezing combination operator, as will be explained later, while S_1 and S_2 are two single-mode squeezing operators [3, 8]. Using IWOP we perform the integrations in (18) to obtain normally ordered forms of V and S_1S_2, respectively,

$$\begin{gathered} S_1 = \exp[-\tfrac{1}{2}a_\xi^{\dagger 2}\tanh\lambda] :\exp[(\operatorname{sech}\lambda - 1)a_\xi^\dagger a_\xi] :\exp[\tfrac{1}{2}a_\xi^2\tanh\lambda]\operatorname{sech}\tfrac{1}{2}\lambda \\ \tanh\lambda = \frac{\sqrt{A}-\sqrt{\mu_1}}{\sqrt{A}+\sqrt{\mu_1}} \end{gathered} \tag{19}$$

$$\begin{gathered} S_2 = \exp[-\tfrac{1}{2}a_\eta^{\dagger 2}\tanh\sigma] :\exp[(\operatorname{sech}\sigma - 1)a_\eta^\dagger a_\eta] :\exp[\tfrac{1}{2}a_\eta^2\tanh\sigma]\operatorname{sech}^{1/2}\sigma \\ \tanh\sigma = \frac{\sqrt{B}-\sqrt{\mu_2}}{\sqrt{B}+\sqrt{\mu_2}} \end{gathered} \tag{20}$$

$$\begin{aligned} V = \iint_{-\infty}^{\infty} & \mathrm{d}\xi\,\mathrm{d}\eta\,|\xi\cos\alpha - \eta\sin\alpha\rangle_{\mu_1\omega_1}|\xi\sin\alpha + \eta\cos\alpha\rangle_{\mu_2\omega_2\mu_2\omega_2}\langle\eta|_{\mu_1\omega_1}\langle\xi| \\ &= \frac{\sqrt{\mu_1\omega_1\mu_2\omega_2}}{\pi\hbar}\iint_{-\infty}^{\infty}\mathrm{d}\xi\,\mathrm{d}\eta :\exp\left\{-\frac{\mu_1\omega_1}{2\hbar}(\xi\cos\alpha-\eta\sin\alpha)^2\right. \\ &\quad + \sqrt{\frac{2\mu_1\omega_1}{\hbar}}(\xi\cos\alpha - \eta\sin\alpha)a_\xi^\dagger \\ &\quad -\frac{1}{2}a_\xi^{\dagger 2} - \frac{\mu_1\omega_1}{2\hbar}\xi^2 - a_\xi^\dagger a_\xi + \sqrt{\frac{2\mu_1\omega_1}{\hbar}}\xi a_\xi - \frac{1}{2}a_\xi^2 \\ &\quad -\frac{\mu_2\omega_2}{2\hbar}(\xi\sin\alpha+\eta\cos\alpha)^2 - \frac{1}{2}a_\eta^{\dagger 2} \\ &\quad +\sqrt{\frac{2\mu_2\omega_2}{\hbar}}(\xi\sin\alpha+\eta\cos\alpha)a_\eta^\dagger - \frac{\mu_2\omega_2}{2\hbar}\eta^2 \\ &\quad \left. +\sqrt{\frac{2\mu_2\omega_2}{\hbar}}\eta a_\eta - \frac{1}{2}a_\eta^2 - a_\eta^\dagger a_\eta\right\}: \\ &= \frac{2}{\sqrt{L}}\exp\left\{\frac{1}{2L}\left[\sin^2\alpha\frac{\mu_1-\mu_2}{\sqrt{\mu_1\mu_2}}(a_\xi^{\dagger 2} - a_\eta^{\dagger 2}) + 2\sin 2\alpha\frac{\sqrt{\mu_2}-\sqrt{\mu_1}}{(\mu_1\mu_2)^{1/4}}a_\xi^\dagger a_\eta^\dagger\right]\right\} \\ &\quad :\exp\left\{(a_\xi^\dagger a_\eta^\dagger)(f - \mathbb{1})\begin{pmatrix}a_\xi\\ a_\eta\end{pmatrix}\right\}: \\ &\quad \times\exp\left\{\frac{1}{2L}\left[\sin^2\alpha\frac{\mu_1-\mu_2}{\sqrt{\mu_1\mu_2}}(a_\xi^2 - a_\eta^2) - 2\sin 2\alpha\frac{\sqrt{\mu_2}-\sqrt{\mu_1}}{(\mu_1\mu_2)^{1/4}}a_\xi a_\eta\right]\right\} \end{aligned} \tag{21}$$

where

$$f=\frac{2}{L}\begin{pmatrix} 2\cos\alpha & -\sin\alpha(\sqrt{\mu_1}+\sqrt{\mu_2})/[(\mu_1\mu_2)^{1/4}] \\ \sin\alpha(\sqrt{\mu_2}+\sqrt{\mu_1})/[(\mu_1\mu_2)^{1/4}] & 2\cos\alpha \end{pmatrix}$$

$$L=2\cos^2\alpha+\sin^2\alpha\frac{\mu_1+\mu_2}{(\mu_1\mu_2)^{1/2}}+2 \qquad \mathbb{1}=\begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}. \tag{22}$$

3. The correctness of the identification of U

We will now prove what we mentioned in the introduction. Using the operator identity [9]

$$:\exp\left\{(a_\xi^\dagger a_\eta^\dagger)(f-\mathbb{1})\begin{pmatrix}a_\xi\\ a_\eta\end{pmatrix}\right\}:=\exp\left[(a_\xi^\dagger a_\eta^\dagger)\ln f\begin{pmatrix}a_\xi\\ a_\eta\end{pmatrix}\right]\equiv W \tag{23}$$

we obtain (note that W is not unitary, but V is)

$$Wa_lW^{-1}=\sum_k (f^{-1})_{lk}a_k \qquad Wa_l^\dagger W^{-1}=\sum_k a_k^\dagger f_{kl} \qquad l,k=(\xi \text{ or } \eta). \tag{24}$$

It then follows from equations (21) and (24) that†

$$Va_\xi V^{-1}=\cos\alpha\, a_\xi+\sin\alpha\frac{\sqrt{\mu_1}+\sqrt{\mu_2}}{2(\mu_1\mu_2)^{1/4}}a_\eta+\sin\alpha\frac{\sqrt{\mu_1}-\sqrt{\mu_2}}{2(\mu_1\mu_2)^{1/4}}a_\eta^\dagger \tag{25}$$

$$Va_\eta V^{-1}=\cos\alpha\, a_\eta-\sin\alpha\frac{\sqrt{\mu_1}+\sqrt{\mu_2}}{2(\mu_1\mu_2)^{1/4}}a_\xi+\sin\alpha\frac{\sqrt{\mu_1}-\sqrt{\mu_2}}{2(\mu_1\mu_2)^{1/4}}a_\xi^\dagger \tag{26}$$

which exhibits both rotating and squeezing transformation, as

$$\frac{(\sqrt{\mu_1}+\sqrt{\mu_2})^2}{4\sqrt{\mu_1\mu_2}}-\frac{(\sqrt{\mu_1}-\sqrt{\mu_2})^2}{4\sqrt{\mu_1\mu_2}}=1.$$

Hence we call V the two-mode rotating-squeezing combination operator. On the other hand,

$$S_1a_\xi S_1^{-1}=a_\xi\cosh\lambda+a_\xi^\dagger\sinh\lambda \qquad S_2a_\eta S_2^{-1}=a_\eta\cosh\sigma+a_\eta^\dagger\sinh\sigma. \tag{27}$$

Combining (18) and (25-27) together we obtain

$$Ua_\xi U^{-1}=\cos\alpha\left(a_\xi\frac{\sqrt{A}+\sqrt{\mu_1}}{2(\mu_1A)^{1/4}}+a_\xi^\dagger\frac{\sqrt{A}-\sqrt{\mu_1}}{2(\mu_1A)^{1/4}}\right)+\sin\alpha\left(a_\eta\frac{\sqrt{A}+\sqrt{\mu_2}}{2(\mu_2A)^{1/4}}+a_\eta^\dagger\frac{\sqrt{A}-\sqrt{\mu_2}}{2(\mu_2A)^{1/4}}\right) \tag{28}$$

$$Ua_\eta U^{-1}=\cos\alpha\left(a_\eta\frac{\sqrt{B}+\sqrt{\mu_2}}{2(\mu_2B)^{1/4}}+a_\eta^\dagger\frac{\sqrt{B}-\sqrt{\mu_2}}{2(\mu_2B)^{1/4}}\right)-\sin\alpha\left(a_\xi\frac{\sqrt{B}+\sqrt{\mu_1}}{2(B\mu_1)^{1/4}}+a_\xi^\dagger\frac{\sqrt{B}-\sqrt{\mu_1}}{2(B\mu_1)^{1/4}}\right). \tag{29}$$

† At this point it is worth pointing out that the complicated form of V in equation (21) originates from $\mu_1\omega_1=\sqrt{\mu_1 k}\neq\mu_2\omega_2=\sqrt{\mu_2 k}$. If $\mu_1=\mu_2$, then (21) reduces to the well known pure rotation operator.

It then follows from (28), (29) and (5) that

$$U\xi U^{-1}=\left(\frac{A}{\mu_1}\right)^{1/4}(\xi\cos\alpha+\eta\sin\alpha)$$
$$U\eta U^{-1}=\left(\frac{B}{\mu_2}\right)^{1/4}(\eta\cos\alpha-\xi\sin\alpha) \tag{30}$$

$$UP_\xi U^{-1}=\left(\frac{\mu_1}{A}\right)^{1/4}(P_\xi\cos\alpha+P_\eta\sin\alpha)$$
$$UP_\eta U^{-1}=\left(\frac{\mu_2}{B}\right)^{1/4}(P_\eta\cos\alpha-P_\xi\sin\alpha) \tag{31}$$

which tells us that the U transformation includes not only the rotation but also the squeezing. The factors $(A/\mu_1)^{1/4}$ and $(B/\mu_2)^{1/4}$ are squeezing parameters which originate from the frequency jump $\omega_1\to\omega_A$, $\omega_2\to\omega_B$. Contrasting equation (30) with equation (7) we realize that the transformation U engendered is more complicated, since in equation (7) no indication of squeezing can be seen. Next we prove that the right-hand side of (6) equals

$$\frac{\omega_B}{\omega_2}U\left(\frac{1}{2\mu_2}P_\eta^2+\frac{k}{2}\eta^2\right)U^{-1}+\frac{\omega_A}{\omega_1}U\left(\frac{1}{2\mu_1}P_\xi^2+\frac{K}{2}\xi^2\right)U^{-1}. \tag{32}$$

In fact, in terms of (30) and (31) the right-hand side of (32) is equal to

$$\begin{aligned}&\frac{P_\xi^2}{2}\left(\frac{\omega_A}{\omega_1\sqrt{\mu_1 A}}\cos^2\alpha+\frac{\omega_B}{\omega_2\sqrt{\mu_2 B}}\sin^2\alpha\right)+\frac{K}{2}\xi^2\left(\frac{\omega_A}{\omega_1}\sqrt{\frac{A}{\mu_1}}\cos^2\alpha+\frac{\omega_B}{\omega_2}\sqrt{\frac{B}{\mu_2}}\sin^2\alpha\right)\\
&\quad+\frac{1}{2}P_\eta^2\left(\frac{\omega_A}{\omega_1\sqrt{\mu_1 A}}\sin^2\alpha+\frac{\omega_B}{\omega_2\sqrt{\mu_2 B}}\cos^2\alpha\right)\\
&\quad+\frac{k}{2}\eta^2\left(\frac{\omega_A}{\omega_1}\sqrt{\frac{A}{\mu_1}}\sin^2\alpha+\frac{\omega_B}{\omega_2}\sqrt{\frac{B}{\omega_2}}\cos^2\alpha\right)\\
&\quad+\frac{1}{2}\left(\frac{\omega_A}{\omega_1\sqrt{\mu_1 A}}-\frac{\omega_B}{\omega_2\sqrt{\mu_2 B}}\right)P_\xi P_\eta\sin 2\alpha\\
&\quad+\frac{k}{2}\xi\eta\left(\sqrt{\frac{A}{\mu_1}}\frac{\omega_A}{\omega_1}-\sqrt{\frac{B}{\mu_2}}\frac{\omega_B}{\omega_2}\right)\sin 2\alpha.\end{aligned} \tag{33}$$

Then using (7), (9) and

$$(\mu_2-\mu_1)/\mu_1\mu_2=(m_3-m_1)/m_1m_3,\ \omega_A/\omega_1=(\mu_1/A)^{1/2} \qquad \omega_B/\omega_2=(\mu_2/B)^{1/2}$$

we have

$$\begin{aligned}&\frac{\omega_A}{\omega_1\sqrt{\mu_1 A}}\cos^2\alpha+\frac{\omega_B}{\omega_2\sqrt{\mu_2 B}}\sin^2\alpha=\frac{1}{A}\cos^2\alpha+\frac{1}{B}\sin^2\alpha\\
&\qquad=\frac{1}{\mu_1}+\sin 2\alpha\left(\frac{m_1-m_3}{2m_1m_3}\sin 2\alpha-\frac{1}{m_2}\cos 2\alpha\right)=\frac{1}{\mu_1}\end{aligned} \tag{34}$$

$$\frac{\omega_A}{\omega_1\sqrt{\mu_1 A}}\sin^2\alpha+\frac{\omega_B}{\omega_2\sqrt{\mu_2 B}}\cos^2\alpha=\frac{1}{\mu_2} \qquad \sqrt{\frac{A}{\mu_1}}\frac{\omega_A}{\omega_1}-\sqrt{\frac{B}{\mu_2}}\frac{\omega_B}{\omega_2}=0 \tag{35}$$

$$\sin 2\alpha\left(\frac{\omega_A}{\omega_1\sqrt{\mu_1 A}}-\frac{\omega_B}{\omega_2\sqrt{\mu_2 B}}\right)=\sin 2\alpha\left(\frac{1}{A}-\frac{1}{B}\right)$$

$$=\sin 2\alpha\left(\cos 2\alpha\frac{m_3-m_1}{m_1 m_3}-\frac{2}{m_2}\sin 2\alpha\right)=-\frac{2}{m_2}. \tag{36}$$

Substituting (34)–(36) into (33) we complete the proof. Because the right-hand side of (32) is just $(\omega_A U(a_\xi^\dagger a_\xi+\frac{1}{2})U^{-1}+\omega_B U(a_\eta^\dagger a_\eta+\frac{1}{2})U^{-1}]\hbar$, we conclude that U indeed engenders the transformation $U|n_1 n_2\rangle=|n_1 n_2\rangle'$. A unitary operator for four-coupled identical oscillators is found in [10].

4. Obtaining the wavefunction by using equation (12)

The coordinate representation of U provides us with a convenient approach to deriving the wavefunction $\langle\xi,\eta|n_1 n_2\rangle'$. Using (12) we have

$$\begin{aligned}
\langle\xi,\eta|n_1 n_2\rangle' &= \int\int_{-\infty}^{\infty}\mathrm{d}\xi'\,\mathrm{d}\eta'\left\langle\begin{pmatrix}\xi\\ \eta\end{pmatrix}\middle|u\begin{pmatrix}\xi'\\ \eta'\end{pmatrix}\right\rangle\left\langle\begin{pmatrix}\xi'\\ \eta'\end{pmatrix}\middle|n_1 n_2\right\rangle\left(\frac{\mu_1\mu_2}{AB}\right)^{1/8}\\
&=\int\int_{-\infty}^{\infty}\mathrm{d}\xi'\,\mathrm{d}\eta'\,\delta\left[\begin{pmatrix}\xi\\ \eta\end{pmatrix}-u\begin{pmatrix}\xi'\\ \eta'\end{pmatrix}\right]\left\langle\begin{pmatrix}\xi'\\ \eta'\end{pmatrix}\middle|n_1 n_2\right\rangle\left(\frac{\mu_1\mu_2}{AB}\right)^{1/8}\\
&={}_{\mu_1\omega_1}\left\langle\left(\frac{A}{\mu_1}\right)^{1/4}(\xi\cos\alpha+\eta\sin\alpha)\middle|n_1\right\rangle\\
&\quad\times{}_{\mu_2\omega_2}\left\langle\left(\frac{B}{\mu_2}\right)^{1/4}(-\xi\sin\alpha+\eta\cos\alpha)\middle|n_2\right\rangle\left(\frac{AB}{\mu_1\mu_2}\right)^{1/8}\\
&=\left[\left(\frac{Ak}{\hbar^2}\right)^{1/4}\frac{1}{\sqrt{\pi}\,2^{n_1}n_1!}\right]^{1/2}\left[\left(\frac{Bk}{\hbar^2}\right)^{1/4}\frac{1}{\sqrt{\pi}\,2^{n_2}n_2!}\right]^{1/2}\\
&\quad\times\exp\left[-\frac{\sqrt{kA}}{2\hbar}(\xi\cos\alpha+\eta\sin\alpha)^2-\frac{\sqrt{kB}}{2\hbar}(-\xi\sin\alpha+\eta\cos\alpha)^2\right]\\
&\quad\times H_{n_1}\left[\left(\frac{Ak}{\hbar^2}\right)^{1/4}(\xi\cos\alpha+\eta\sin\alpha)\right]H_{n_2}\left[\left(\frac{Bk}{\hbar^2}\right)^{1/4}(-\xi\sin\alpha+\eta\cos\alpha\right]
\end{aligned} \tag{37}$$

where H_n is the Hermite polynomial, and we have used

$${}_{\mu_1\omega_1}\langle\xi|n_1\rangle=\left(\frac{\mu_1\omega_1}{\pi\hbar}\right)^{1/4}(2^{n_1}n_1!)^{-1/2}\exp\left[-\frac{\mu_1\omega_1}{2\hbar}\xi^2\right]H_{n_1}\left(\sqrt{\frac{\mu_1\omega_1}{\hbar}}\,\xi\right)$$

$${}_{\mu_2\omega_2}\langle\eta|n_2\rangle=\left(\frac{\mu_2\omega_2}{\pi\hbar}\right)^{1/4}(2^{n_2}n_2!)^{-1/2}\exp\left[-\frac{\mu_2\omega_2}{2\hbar}\eta^2\right]H_{n_2}\left(\sqrt{\frac{\mu_2\omega_2}{\hbar}}\,\eta\right).$$

In summary, we have found the frequency-jump related unitary operator for the triatomic linear molecule. This U, together with the IWOP technique provides a new approach to studying the dynamics of this molecule. The extension of this approach, to study bending vibrations of the molecule or other more complicated molecules, is expected.

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