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Dynamics of bipartite vibrational entanglement under the inherent decoherence process in H_2O

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Abstract. In present study, the dynamics of stretching-stretching and stretching-bending entanglement in H_2O are studied with considering the inherent decoherence process. It is shown that the excitation in the bending vibration can lead to the decrease of the generation rate of stretching-stretching entanglement for the non-superposed state and the degeneration of entanglement for the initial entangled states. For specific initial entangled states, the stretching-stretching entanglement can live for a long time, and the correspondence between energy transfer and entanglement is still maintained for the initial local mode states. For the stretching-bending vibrations, the stretching-bending entanglement is much lower than the stretching-stretching vibration, and the degeneration rate of stretching-bending entanglement is higher than that of the stretching-stretching entanglement. The excitation in the remaining stretching vibration can induce a higher degree of stretching-bending entanglement.

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Key words: bipartite vibrational entanglement, inherent decoherence process, Lie algebraic method for molecular vibration.

1 Introduction

As a unique feature of quantum mechanics, entanglement is a valuable resource for a number of quantum information processing [1–6]. Some investigative efforts have been focused on the study of dynamical properties entanglement in different systems [7–9]. Over past few years, the feasibility of using molecular vibrational modes as one candidate for quantum computing has been suggested by many researchers [10–13]. In the

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molecular system, there are dense quantum vibrational states which can be manipulated by the laser fields, and the extremely high fidelity quantum gates can be constructed based on vibrational eigenstates. Moreover, recent study has demonstrated that the entanglement and arbitrary superposition states of molecular vibrations can be generated and controlled by using sequential chirped pulses [14]. Because of the importance of dynamical properties of entanglement [7, 15, 16], the entanglement of vibrations in the molecular systems have attracted much attention recently [17–24].

The bipartite entanglement dynamics in the small molecular systems were investigated in many aspects, such as, entanglement between the electronic and vibrational freedoms [18, 19], the dynamics of entanglement between two vibrational modes [20–25] etc. As the simplest polyatomic molecule, the triatomic molecule is often chosen as the prototype in the investigations of entanglement dynamics of vibrations. In the local mode description, there are two stretching and one bending vibrations in a triatomic molecule. Two type bi-qubit systems could be established, i.e., the stretching-stretching (SS) and stretching-bending (SB) system. Recently, the SS entanglement in the triatomic molecules were studied frequently. The dynamical properties of SS entanglement have been investigated in different type triatomic molecules including the local mode (LM) symmetrical molecule, normal mode (NM) symmetrical molecule and the non-symmetrical linear triatomic molecules [20,22,23]. The relations between the entanglement and energy transfer and the underlying classical chaos are explored [23], and the mean SS entanglement was employed to label the normal-to-local transition [25]. However, there are seldom works have been done to study the dynamics of SS vibrational entanglement under the decoherence process and the dynamical properties of SB entanglement.

For the molecular vibrational qubits, the decoherence resources may come from the collisions with other molecules and the intramolecular anharmonic resonances. Regarding molecules in the gas phase, the number of collisions can be kept low. Therefore, the main resource of decoherence of the vibrational qubits is from the remaining vibrational modes. For the SS qubit system in the triatomic molecule, the bending vibration can lead to the decoherence, while the remaining stretching vibration is the main decoherence resource of the SB qubit system. Since decoherence can lead to the degradation of entanglement [26], the studies on the dynamical properties of vibrational entanglement under the decoherence process are thus meaningful in selecting suitable vibration to apply quantum computation, controlling decoherence and protecting entanglement [20, 23, 27, 28]. In present study, the dynamical properties of SS and SB entanglement in a triatomic LM molecule H_2O are investigated. To do this, a Lie algebraic method for the vibrations in molecules is employed to construct the vibrational Hamiltonian in the LM description. Based on this model, the stretching and bending vibrations are well described, and the vibrational spectroscopy can be explicitly reproduced with few parameters. Therefore, such study could be regarded as an alternative with the potential connections to actual experiments.

The paper is organized as follows. In Sec. 2, the vibrational Hamiltonian of triatomic molecule is constructed, and the measurements of SS and SB entanglement are presented.

In Sec. 3, the numerical results of dynamics of SS and SB entanglement are presented, and the influences of decoherence on dynamical entanglement are also investigated. Finally, a briefly discussion and conclusion are presented in Sec. 4.

2 Theoretical framework

Lie algebraic method for molecules has shown to be efficient in describing the ro-vibrational spectra and vibrational dynamics of polyatomic molecules [21,29–33]. In this paper, the $U(4)$ algebra is introduced for each bond of the triatomic molecule to describe its 3 degrees of freedom [30], and the symmetric group is $U_1(4)\otimes U_2(4)$. Following the dynamical symmetries, the algebra admits two subalgebra chains [30,31]:

$$\begin{aligned}&U_1(4)\otimes U_2(4)\supset U_{12}(4)\supset O_{12}(4),\\&U_1(4)\otimes U_2(4)\supset O_1(4)\otimes O_2(4)\supset O_{12}(4).\end{aligned}\tag{1}$$

In terms of Casimir operators of subgroups, the Hamiltonian operator of ro-vibrations of triatomic molecules can be constructed as [30]:

$$\mathcal{H}=A_1C_1+A_2C_2+A_{12}C_{12}^{(1)}+A'_{12}C_{12}^{(2)}+\lambda M_{12},\tag{2}$$

where A_1, A_2, A_{12}, A'_{12} and λ are the expansion coefficients. C_1 and C_2 are Casimir operators of groups $O_1(4)$ and $O_2(4)$ respectively; $C_{12}^{(1)}$ and $C_{12}^{(2)}$ are two Casimir operators of $O_{12}(4)$; M_{12} is the Majorana operator denoting the coupling between two bonds.

The local basis is characterized by

$$|[N_1][N_2](\omega_1,0)(\omega_2,0)(\tau_1,\tau_2)\rangle,\tag{3}$$

where $[N_i]$ labels the total symmetric representation of $U_i(4)$ $(i=1,2)$, $(\omega_i,0)$ labels the symmetric representation of $O_i(4)$ $(i=1,2)$, and (τ_1,τ_2) denotes the irreducible representation of $O_{12}(4)$. Physically, N_i characterizes the total number of bosons in bond i [34].

The value of ω_i is taken as

$$\omega_i=\begin{cases}N_i,N_i-2,\ldots,1, & \text{if } N_i \text{ is odd;}\\ N_i,N_i-2,\ldots,0, & \text{if } N_i \text{ is even.}\end{cases}\tag{4}$$

By denoting the quantum numbers of two stretching, bending vibations and rotation as v_1, v_2, v_b and κ respectively, the relations between $(\omega_1,\omega_2,\tau_1,\tau_2)$ and (v_1,v_b,v_2,κ) are as follows [30]:

$$\begin{aligned}&v_1=\frac{1}{2}(N_1-\omega_1),\\&v_2=\frac{1}{2}(N_2-\omega_2),\\&v_b=\frac{1}{2}(\omega_1+\omega_2-\tau_1-\tau_2),\\&\kappa=\tau_2.\end{aligned}\tag{5}$$

Under the local basis of Eq.(3), the matrix elements of the operators C_1,C_2,$C_{12}^{(1)}$ and $C_{12}^{(2)}$ are as follows:

$$\begin{aligned}
&\langle C_1\rangle = (N_1-2v_1)(N_1-2v_1+2),\\
&\langle C_2\rangle = (N_2-2v_2)(N_2-2v_2+2),\\
&\langle C_{12}^{(1)}\rangle = (N_{12}-2v-\kappa)(N_{12}-2v-\kappa+2)+\kappa^2,\\
&\langle C_{12}^{(2)}\rangle = (N_{12}-2v-\kappa)\kappa,
\end{aligned} \tag{6}$$

where $N_{12}=N_1+N_2$ and $v=v_1+v_2+v_b$. The matrix elements of M_{12} can be calculated as [34]:

$$\begin{aligned}
&\langle N_1N_2\omega_1\omega_2(\tau_1,\tau_2)|M_{12}|N_1N_2\omega_1\omega_2(\tau_1,\tau_2)\rangle\\
=&\frac{3}{4}N_1N_2-\frac{1}{4}\{\tau_1(\tau_1+\tau_2+2)-\omega_1(\omega_1+2)-\omega_2(\omega_2+2)\}\\
&-\frac{(N_1+2)(N_2+2)}{16\omega_1(\omega_1+2)\omega_2(\omega_2+2)}\\
&\times[\omega_1(\omega_1+2)+\omega_2(\omega_2+2)-(\tau_1+\tau_2)(\tau_1+\tau_2+2)]\\
&\times[\omega_1(\omega_1+2)+\omega_2(\omega_2+2)-(\tau_1-\tau_2)(\tau_1-\tau_2+2)],
\end{aligned} \tag{7}$$

and

$$\begin{aligned}
&\langle N_1N_2\omega_1'\omega_2'(\tau_1,\tau_2)|M_{12}|N_1N_2\omega_1\omega_2(\tau_1,\tau_2)\rangle\\
=&(-1)^{\tau_1+1}(\omega_1'+1)(\omega_2'+1)\times\left\{\begin{array}{ccc}\frac{\omega_1}{2} & \frac{\omega_2}{2} & \frac{\tau_1-\tau_2}{2}\\ \frac{\omega_1'}{2} & \frac{\omega_2'}{2} & 1\end{array}\right\}\\
&\times\left\{\begin{array}{ccc}\frac{\omega_1}{2} & \frac{\omega_2}{2} & \frac{\tau_1+\tau_2}{2}\\ \frac{\omega_1'}{2} & \frac{\omega_2'}{2} & 1\end{array}\right\}\langle N_1\omega_1'||\hat{D}_1||N_1\omega_1\rangle\\
&\langle N_2\omega_2'||\hat{D}_2||N_2\omega_2\rangle\delta_{\omega_1',\omega_1\pm2}\delta_{\omega_1',\omega_1\pm2},
\end{aligned} \tag{8}$$

where $\{\cdots\}$ is the Wigner $6-j$ symbol. The matrix elements of $\langle N\omega'||\hat{D}||N\omega\rangle$ are given as

$$\langle N\omega'||\hat{D}||N\omega\rangle=\begin{cases}\frac{N+2}{2} & \omega'=\omega\\ \frac{1}{2}\sqrt{\frac{(N-\omega+2)(N+\omega+2)(\omega+1)}{\omega-1}} & \omega'=\omega-2\\ \frac{1}{2}\sqrt{\frac{(N-\omega)(N+\omega+4)(\omega+1)}{\omega+3}} & \omega'=\omega+2\end{cases}. \tag{9}$$

Although the rotational motion can lead to the decoherence of vibrations, molecular rotational transitions in excited vibrational states are generally very weak. The rotational motion is thus neglected, namely, we assume $\kappa=0$. The expansion coefficients in Eq.(2) of H_2O, obtained by fitting its vibrational spectra in Ref. [33], are $A_1=A_2=-18.2219$ cm^{-1}, $A_{12}=-2.85$ cm^{-1}, $\lambda=1.0571$ cm^{-1}, and $N_1=N_2=42$.

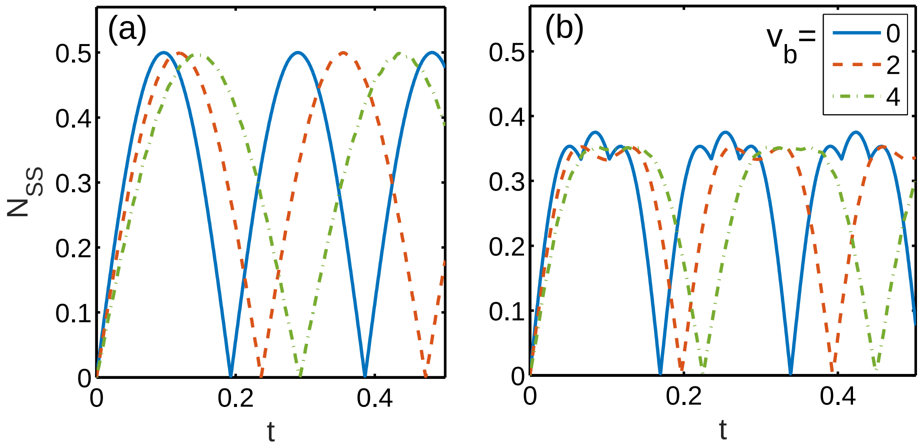

Figure 1: The dynamics of $\mathcal{N}_{SS}$ with (a) $|\psi_{SS}(0)\rangle = |0,1\rangle$ and (b) $|\psi_{SS}(0)\rangle = |1,1\rangle$. $v_b = 0$, 2 and 4. Time t is in ps.

The negativity is employed to measure the bipartite entanglement under decoherence, which is defined as [35]

$$\mathcal{N} = \max(0, -\mu_{min}) \tag{10}$$

where μ_{min} is the minimum value of the eigenvalues of the partial transpose $\sigma(t)$. The partial transpose $\sigma(t)$ of the density matrix $\rho(t)$ can be calculated by

$$\sigma_{i\beta,j\alpha}(t) = {}^{T_2}\rho_{i\alpha,j\beta}(t), \tag{11}$$

where T_2 represents the partial transpose in density matrix $\rho(t)$ for the second subsystem. The negativity of SS vibrations and SB vibrations are noted as $\mathcal{N}_{SS}$ and $\mathcal{N}_{SB}$, respectively.

3 Numerical results

3.1 The dynamics of SS entanglement

We discuss the dynamics of SS entanglement for the case that the bending vibration and SS vibrations are initially separable. The initial state is written as

$$|\psi(0)\rangle = |\psi_{SS}(0)\rangle \otimes |v_b\rangle, \tag{12}$$

where $|\psi_{SS}(0)\rangle$ is the initial state of SS vibrations, and $|v_b\rangle$ is the initial state of bending motion. Since the ground state and first-excited state are usually taken to represent the qubit, the dynamics of $\mathcal{N}_{SS}$ with states of $v_{1(2)} = 0,1$ are firstly studied. Noting that $|v_1, v_2\rangle \equiv |v_1\rangle \otimes |v_2\rangle$, $|\psi_{SS}(0)\rangle$ takes *four* different states: $|0,1\rangle$ (for the SS vibration of H_2O, the dynamics of initial state $|1,0\rangle$ are identical with $|0,1\rangle$), $|1,1\rangle$, $|0,1\rangle + |1,0\rangle$ and

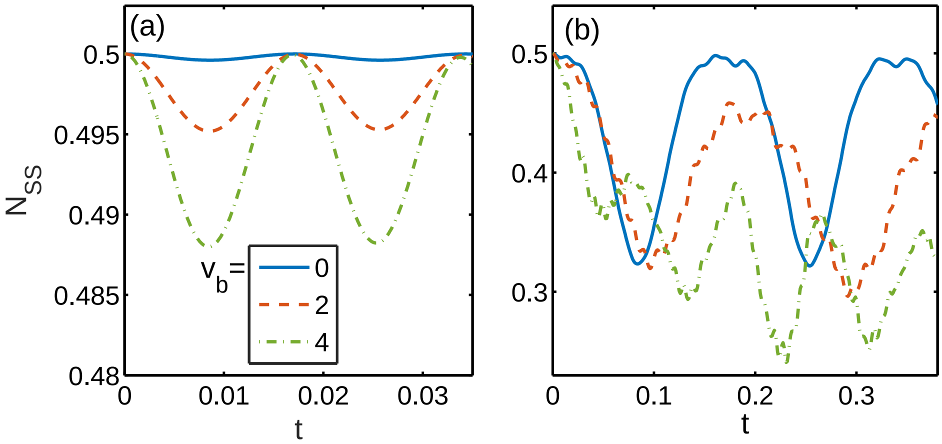

Figure 2: The dynamics of $\mathcal{N}_{SS}$ with (a) $|\psi_{ss}(0)\rangle = |0,1\rangle + |1,0\rangle$ and (b) $|\psi_{SS}(0)\rangle = |0,0\rangle + |1,1\rangle$ with $v_b = 0,2$ and 4. Time t is in ps.

$|0,0\rangle + |1,1\rangle$ (hereafter, the normalization constant is neglected). v_b is set to different values to study its influences on SS entanglement.

In Fig. 1, $\mathcal{N}_{SS}$ as functions of time t for $|\psi_{SS}(0)\rangle = |0,1\rangle$ and $|1,1\rangle$ are plotted. v_b is set to 0, 2 and 4. As demonstrated in the previous study, the bipartite entanglement between two stretching vibrations could be generated dynamically for a initial separable state, and its dynamical behavior was highly depended on the the energy change between vibrations [23]. For the low excited states, the energy transfer between vibrations is periodical [36]. As a result, from Fig. 1, it is found that both the $\mathcal{N}_{SS}$ of $\psi_{SS}(0) = |01\rangle$ and $|1,1\rangle$ are varying from disentanglement to its maximum value periodically. With the increase of v_b, the period of energy transfer will extend, and the period of $\mathcal{N}_{SS}$ becomes longer correspondingly. Since more states are involved in the evolution, the $\mathcal{N}_{SS}$ becomes irregular. Another influence of bending vibration is that the maximum values of $\mathcal{N}_{SS}$ decrease with the increase of v_b. Such behaviors of $\mathcal{N}_{SS}$ show that the bending vibration can reduce the generation rate of entanglement.

For the case of initial superposition states: $|\psi_{SS}(0)\rangle = |0,1\rangle + |1,0\rangle$ and $|0,0\rangle + |1,1\rangle$, the dynamics of $\mathcal{N}_{SS}$ are plotted in Fig. 2. During the vibration, the total vibrational quantum number v is invariable for the initial state $|0,1\rangle + |1,0\rangle$, and only the states corresponding to v will be involved. Therefore, the decoherence caused by the bending vibration is not very serious. Without the decoherence process from the bending vibration, the $|0,1\rangle + |1,0\rangle$ is one eigenstate of the SS vibrations, so that, the $\mathcal{N}_{SS}$ keeps its maximum value during evolution. The influence from bending vibration is directly demonstrated as the decrease of $\mathcal{N}_{SS}$ as shown in Fig. 2 (a). We can find that $\mathcal{N}_{SS}$ evolves periodically in a high degree of entanglement. The minimal value of $\mathcal{N}_{SS}$ decreases with the increase of v_b, but the period is almost invariable. The result shows that the increase of the initial excitation in bending vibration promotes the degeneration rate of entangle-

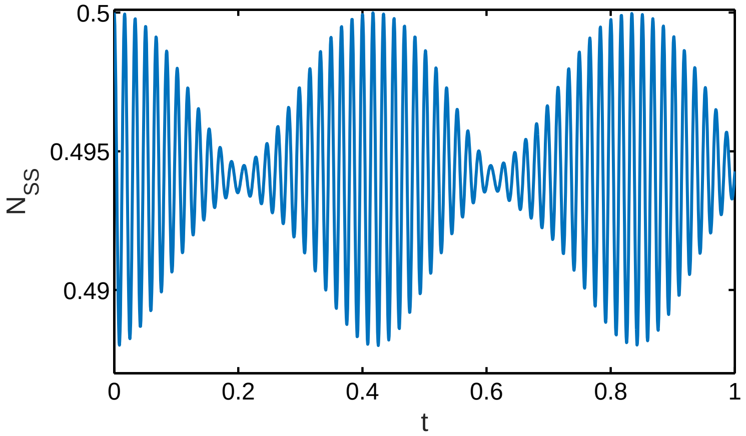

Figure 3: The dynamics of $\mathcal{N}_{SS}$ with $|\psi_{SS}(0)\rangle=|0,1\rangle+|1,0\rangle$ and $v_b=4$. Time t is in ps.

ment. Moreover, it should be noted that in the long-time evolution, the dynamic of $\mathcal{N}_{SS}$ of $|\psi_{SS}(0)\rangle=|0,1\rangle+|1,0\rangle$ with $v_b=4$ shows the beat phenomenon as shown in Fig. 3, which means the high degree of entanglement can hold a long time. Similar beat phenomenon has also been found in the LM vibrations in LM molecules and other systems [23, 37], which is demonstrated as the carrier of information.

For the initial state $|\psi_{SS}(0)\rangle=|0,0\rangle+|1,1\rangle$, v is not persevered during the vibration, and the states corresponding to v varying from v_b to v_b+2 are involved in the vibration. As a result, the decoherence process is significant. With $v_b=0$, $\mathcal{N}_{SS}$ of $|\psi_{SS}(0)\rangle=|0,0\rangle+|1,1\rangle$ evolves periodically as shown in Fig. 2 (b). However, the periodical evolution of $\mathcal{N}_{SS}$ is destroyed with $v_b=2$ and 4. Comparing with the initial state $|0,1\rangle+|1,0\rangle$, the variation amplitude of $\mathcal{N}_{SS}$ of $|0,0\rangle+|1,1\rangle$ is much greater, which means the entanglement is destroyed more significant. The resuts of $\mathcal{N}_{SS}$ of $|\psi_{SS}(0)\rangle=|0,1\rangle+|1,0\rangle$ and $|0,0\rangle+|1,1\rangle$ show that the bending vibration can induce to the destruction of entanglement between the stretching vibrations. However, when bending vibration is not highly excited, the $\mathcal{N}_{SS}$ can recover to the high degree of entanglement periodically, which could be used in the quantum computing. Moreover, the destruction of entanglement is not serious comparing with the bipartite entanglement in the NM molecule SO_2 studied in [24], and the reason is because the coupling between vibration is strong in the normal mode molecules.

For the LM molecule, the dynamical behaviors of stretching-stretching entanglement of initial LM states (one of the stretching vibrations is firstly excited) were significantly different from the initial NM states (two stretching vibration are initially excited equally). It was found that the entanglement of LM states forms a long-time sine wave, and the entanglement has a clear relation with the energy transfer between vibrations which is exhibited as the maximum of entanglement appears only around $E_{s1}=E_{s2}$, where E_{si} is the energy of stretching vibration of bond i. In Fig. 4, the $\mathcal{N}_{SS}$ of the LM state $|0,4\rangle$ and

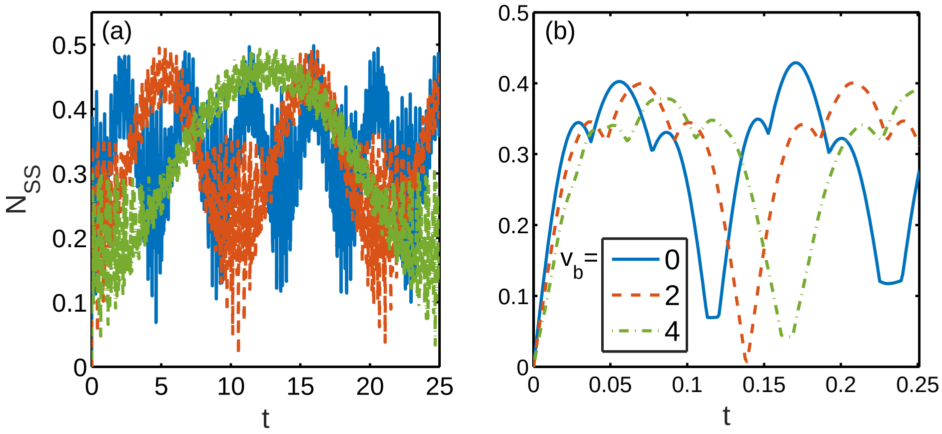

Figure 4: The dynamics of $\mathcal{N}_{SS}$ with (a) $|\psi_{SS}(0)\rangle=|0{,}4\rangle$ and (b) $|\psi_{SS}(0)\rangle=|2{,}2\rangle$. Time t is in ps.

NM state $|2{,}2\rangle$ with v_b=0,2 and 4 are plotted. It is clear that the $\mathcal{N}_{SS}$ of the LM state is also shown as the long-period sine-like wave in Fig. 4 (a). With the increase of v_b, the period is extended extensively. However, the correspondence between the energy transfer and $\mathcal{N}_{SS}$ still maintain. As shown in Fig. 5, the shape of $\Delta E \sim \mathcal{N}_{SS}$ of $|\psi_{SS}(0)\rangle=|0{,}4\rangle$ and $v_b=4$ is plotted, where $\Delta E=(E_{s1}-E_{s2})/E$ and E is total energy. It is clear that the maximum of $\mathcal{N}_{SS}$ still appear at $\Delta E=0$, which means the $\mathcal{N}_{SS}$ of the LM state strongly depends on the energy transfer between the vibrations. Therefore, the extension of the period could be easily understood because the excitation in bending vibration leads to the increase of involved Fock states during evolution. The distance between two LM characteristic states increases with v_b, thus the period of completely energy exchange between modes is extended observably. For the NM state $|2{,}2\rangle$, the energy transfers freely between stretching vibrations, therefore, the $\mathcal{N}_{SS}$ oscillators periodically with a short period, which is similar to that of the low excited sates in Fig. 1. With the increase of v_b the period is also extended since the involved states are increased.

3.2 The dynamics of SB entanglement

In this subsection, we assume the SB vibrations and remaining stretching vibration are separable initially, that is, the initial state is taken as follows

$$|\psi(0)\rangle=|\psi_{SB}(0)\rangle\otimes|v_2\rangle. \tag{13}$$

In Fig. 6, the dynamical natures of $\mathcal{N}_{SB}$ of initial states $|\psi_{SB}(0)\rangle=|1{,}0\rangle$, $|0{,}1\rangle$ and $|1{,}1\rangle$ are plotted, where $|v_1{,}v_b\rangle=|v_1\rangle\otimes|v_b\rangle$. Due to the weak coupling of SB vibrations, $\mathcal{N}_{SB}$ is much smaller than $\mathcal{N}_{SS}$. For $v_2=0$, the evolution of $\mathcal{N}_{SB}$ of $|\psi_{SB}\rangle=|0{,}1\rangle$ is periodical, which is different from the other two states. However, with the increase of v_2, the periodical evolution is totally destroyed. Such behavior can attribute to the fact that SS coupling

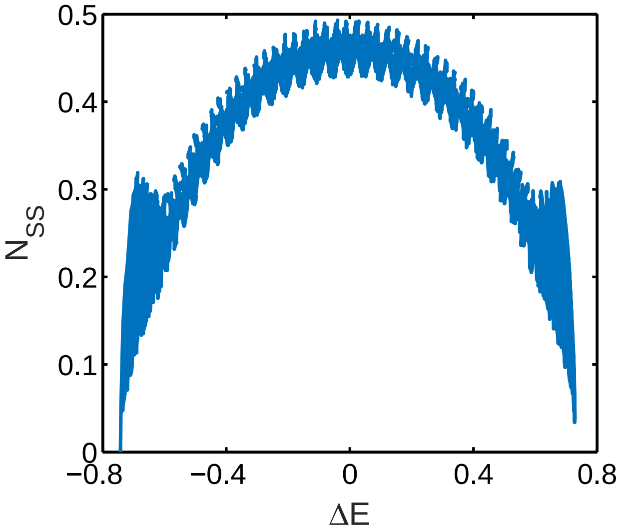

Figure 5: The shape of $\Delta E \sim \mathcal{N}_{SS}$ for $|\psi_{SS}(0)\rangle = |0,4\rangle$ and $v_b = 4$. Time t is in ps.

is much stronger than SB coupling. The energy exchange is mainly happened between SS vibrations which makes the dynamical behaviors of $\mathcal{N}_{SB}$ are totally different. The results demonstrate that the remaining stretching vibration is of significant effect, and energy transfer path of SS vibrations play a vital role in the dynamics of SB entanglement. Moreover, with the increase of v_2, the achieved maximum entanglement is enhanced, and the peak values increase with the growth of v_2 (the results for even higher values of v_2 are not shown here). Such phenomenon indicates that the remaining stretching vibration can improve the SB entanglement. The appearance of the outstand pick in the $\mathcal{N}_{SB}$ curve is also determined by the energy flow between SS vibrations, which means the high degree of SB entanglement can also be achieved by controlling the energy exchange between stretching vibrations. Although not shown here, $\mathcal{N}_{SB}$ of the high excited LM and NM states, e.g., $|\psi_{SB}(0)\rangle = |0,4\rangle, |4,0\rangle$ and $|2,2\rangle$, have the similar dynamical behavior with $|\psi_{SB}(0)\rangle = |0,1\rangle, |1,0\rangle$ and $|1,1\rangle$.

The $\mathcal{N}_{SB}$ of $|\psi_{SB}(0)\rangle = |0,1\rangle + |1,0\rangle$ and $|0,0\rangle + |1,1\rangle$ are plotted in Fig. 7. For these initial states, the decoherence from the remaining stretching vibration is also remarkable. When $v_2 = 0$, the negativity $\mathcal{N}_{SB}$ varies periodically with a large amplitude, which means the remaining stretching vibration can induce a significant degeneration of $\mathcal{N}_{SB}$. With the growth of v_2, the variation of $\mathcal{N}_{SB}$ becomes irregular. Early study had found that the $\mathcal{N}_{SB}$ in the NM molecule can recover to the maximum entanglement periodically under the decoherence from the remaining stretching vibration [24]. The difference between the behaviours of $\mathcal{N}_{SB}$ of LM and NM molecules may lie in the SB coupling in the NM molecule is much larger than that in the LM molecules.

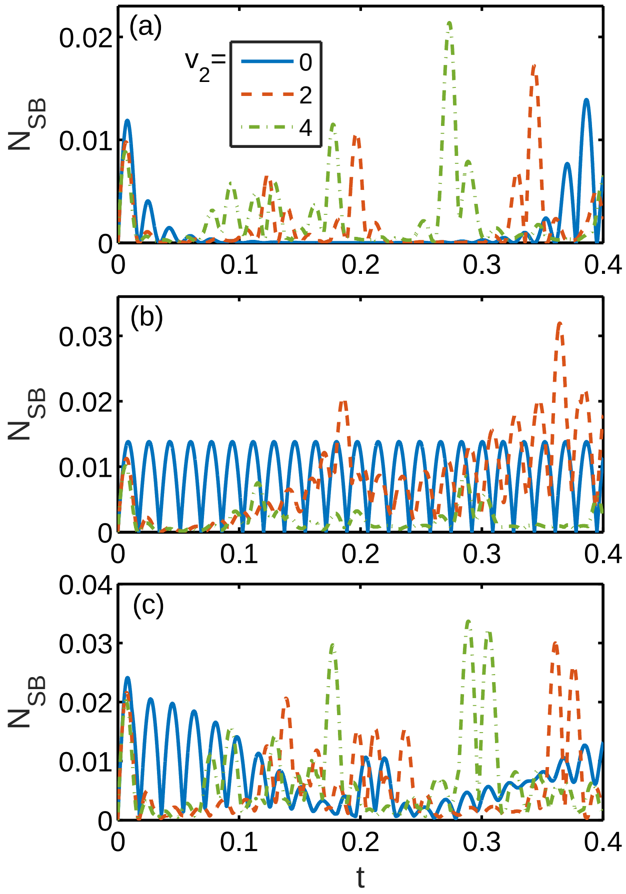

Figure 6: The dynamics of $\mathcal{N}_{SB}$ with (a) $|\psi_{SB}(0)\rangle=|1,0\rangle$, (b) $|\psi_{SB}(0)\rangle=|0,1\rangle$ and (c) $|\psi_{SB}(0)\rangle=|1,1\rangle$ with $v_2=0,2$, and 4. Time t is in ps.

4 Conclusions

In this paper, the entanglement of SS and SB vibrations in the H_2O are studied. Our investigation shows that if the bi-qubit system is initially in a non-superposed state, SS vibrations can achieve a higher degree of entanglement comparing with the SB vibrations. If the bi-qubit system is initially in the entangled state, the degeneration rate of SB entanglement is higher than that of the SS entanglement. From the results of both non-superposed and superposition states, the qubit constructed by SS vibrations has great advantages on the robustness of entanglement. Although the strong coupling can leads to the generation of high degree of entanglement for the SB qubit system, the strong coupling between the qubit system and remaining vibration modes should be avoided in constructing qubit subsystem. For the high excited states of the SS vibrations, the dynam-

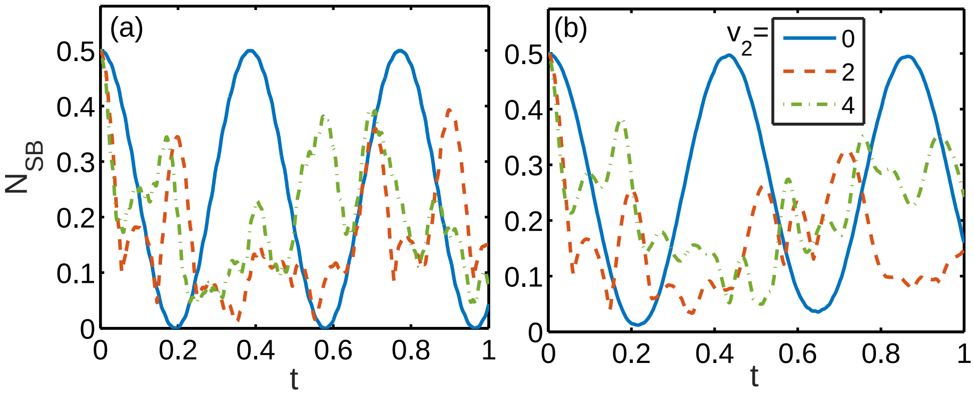

Figure 7: The dynamics of $\mathcal{N}_{SB}$ with (a) $|\psi_{SB}(0)\rangle = |0{,}1\rangle + |1{,}0\rangle$ and (b) $|\psi_{SB}(0)\rangle = |0{,}0\rangle + |1{,}1\rangle$ with $v_2 = 0{,}2$, and 4. Time t is in ps.

ical properties of the initial LM and NM character states also show significant difference. The correspondence between the energy transfer and entanglement is still maintained for the initial LM states, which means the entanglement is still controllable by controlling the energy distribution between different vibrations. From the viewpoints of robustness of entanglement, the SS vibrations are more suitable to construct a bi-qubit system in the LM triatomic molecule. Those results can be useful in experiential realization of molecular vibrational quantum computing.

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