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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.