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Algebraic approach to geometric Quantum Speed Limits in triatomic molecules

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Abstract. The appropriate metric of quantum speed limit for the triatomic molecules is discussed using a generalized geometric approach. The researches show the quantum Fisher information metric is tighter than the Wigner-Yanase information metric in realistic molecular dynamical evolution. The quantum speed limit metric is related to the initial evolution state of molecules.

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Key words: Lie-algebra, quantum speed limit, triatomic molecules.

1 Introduction

The quantum speed limit originates from the time-energy uncertainty relation which is the nature of the quantum mechanics. It represents the maximal evolution speed of a quantum system. With the development of quantum information science and laser technology, dynamical evolutions of quantum system become exceedingly short-timed evolutions, which bring along a practical applicability for the quantum speed limit and the problem has become the focus topic in the current frontier field. The bound of the quantum speed limit time for unitary evolutions in a closed system is firstly given by the Mandelstam and Tamm [1], then Margolus and Levitin provided another QSL (quantum speed limit) on the time evolution which is tighter than MT bound but does not recover the MT one [2]. Later, the MT QSL and ML QSL are extended to be suitable for more dynamical system [3–12]. However, QSL for the realistic molecular system has not been proposed. Recently, Diego Paiva Pires and his co-workers construct a new fundamental family of geometric quantum speed limits [13] and provide the quantity how much a

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certain geometric QSL is saturated. They take single-qubit unitary dynamics as an example and prove that the geometric QSL corresponding to the quantum Fisher information metric is tighter than the one corresponding to the Wigner-Yanase information metric, but they do not give the result if a higher-dimensional quantum system is considered. Here we extend the method to the molecular system and discuss the question whether it is same to the single-qubit system. The algebraic model of the molecule has been applied successfully to study vibrations in polyatomic molecules [14–18], and has been extended to research the dynamical entanglement in small molecules [19, 20].

This paper proceeds as follows. In Sec. 2, the algebraic molecular model is first reviewed briefly, and the geometric quantum speed limits are given using the algebraic model. In Sec. 3, the generalized geometric QSLs corresponding to the the quantum Fisher information metric and the Wigner-Yanase information are calculated, then the relative difference between the dynamical evolution distance and the geodesic is discussed. Finally, concluding remarks are given in Sec. 4.

2 Quantum Speed Limits metric in triatomic molecules

The algebraic Hamiltonian of a free linear triatomic molecule can be represented as two coupled quadratic anharmonic oscillators using the $U(2)$ algebra [21, 22]

$$\hat{H} = \hbar\omega_{01}\left(\hat{A}_1^\dagger\hat{A}_1+\frac{\hat{I}_{01}}{2}\right)+\hbar\omega_{02}\left(\hat{A}_2^\dagger\hat{A}_2+\frac{\hat{I}_{02}}{2}\right)-\lambda(\hat{A}_1^\dagger\hat{A}_2+\hat{A}_2^\dagger\hat{A}_1), \tag{1}$$

where ω_{01} and ω_{02} are the angular frequencies of the triatomic molecule corresponding to the bond 1 and bond 2. λ is the coupling coefficient which depend on the experimental values of realistic molecular spectra. The quadratic operators $\hat{A}_i^\dagger, \hat{A}_i, \hat{I}_{0i}$ act on the state $|N_i, v_i\rangle$ [21],

$$\begin{aligned}
&\hat{A}_i^\dagger|N_i,v_i\rangle = \sqrt{(1-x_{0i}v_i)(v_i+1)}|N_i,v_i+1\rangle\\
&\hat{A}_i|N_i,v_i\rangle = \sqrt{[1-x_{0i}(v_i-1)]v_i}|N_i,v_i-1\rangle\\
&\hat{I}_{0i}|N_i,v_i\rangle = 1-2x_{0i}v_i|N_i,v_i\rangle,
\end{aligned} \tag{2}$$

where $x_{0i}=1/N_i$ is the anharmonic correction [23, 24].

The time-dependent wave function can be written as the following form when the initial states are chosen to be $|\psi(0)\rangle = |N_1,v_1\rangle\otimes|N_2,v_2\rangle \equiv |v_0, v_n - v_0\rangle$,

$$\begin{aligned}
|\psi(t)\rangle &= e^{-it\hat{H}}|\psi(0)\rangle\\
&= e^{-it\hat{H}}|v_0,v_n-v_0\rangle\\
&= \sum_{k=0}^{\infty}\frac{(-it)^k}{k!}\hat{H}^k|v_0,v_n-v_0\rangle
\end{aligned}$$