J. At. Mol. Sci.
doi: 10.4208/jams.062016.081216a

Vol. **7**, No. 4, pp. 207-212
November 2016

Algebraic approach to geometric Quantum Speed Limits in triatomic molecules

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Received 20 June 2016; Accepted (in revised version) 12 August 2016
Published Online 10 November 2016

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.

PACS: 02.20.Sv, 03.67.-a, 33.15-e

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 $|\psi(0)\rangle = |N_1,v_1\rangle\otimes|N_2,v_2\rangle \equiv |v_0, v_n - v_0\rangle$,

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

$$
\begin{aligned}
&= \sum_{k=0}^{\infty} \sum_{max\{-k,-v_0\}}^{min\{k,v_n-v_0\}} \Gamma_k^m(t)|v_0+m,v_n-v_0-m\rangle \\
&= \sum_{m=-v_0}^{v_n-v_0} P^m(t)|v_0+m,v_n-v_0-m\rangle. \qquad (3)
\end{aligned}
$$

where $P^m(t)=\sum_{k=|m|}^{\infty}\Gamma_k^m(t)$. When k=0, $\Gamma_0^m(t)=\delta_{0,m}$, and when k=1,2,3,...,∞, the recursive expression $\Gamma_k^m(t)$ is

$$
\begin{aligned}
\Gamma_k^m(t) = -\frac{it}{k}\cdot\{&\gamma_0(v_0+m,v_n-v_0-m)\Gamma_{k-1}^m(t) \\
&+\gamma_+(v_0+m,v_n-v_0-m)\Gamma_{k-1}^{m+1}(t) \\
&+\gamma_-(v_0+m,v_n-v_0-m)\Gamma_{k-1}^{m-1}(t)\Big\} \qquad (4)
\end{aligned}
$$

in which the function $\gamma_0,\gamma_+,\gamma_-$ can be obtained using algebraic operations

$$
\begin{aligned}
&\gamma_0(v_1,v_2)=\hbar\omega_{01}(v_1^2-x_{01}v_1^2)+\hbar\omega_{02}(v_2^2-x_{02}v_2^2) \\
&\gamma_+(v_1,v_2)=-\lambda\sqrt{(1-x_{01}v_1)(v_1+1)}\cdot\sqrt{[1-x_{02}(v_2-1)]v_2} \\
&\gamma_-(v_1,v_2)=-\lambda\sqrt{[1-x_{01}(v_1-1)]v_1}\cdot\sqrt{(1-x_{02}v_2)(v_2+1)}. \qquad (5)
\end{aligned}
$$

where $v_1=v_0+m,v_2=v_n-v_0-m$.

The analytical expression of reduced-density matrices can be given using the equation (3),

$$
\begin{aligned}
\rho_1(t) &= Tr_2\rho(t) \\
&= Tr_2\{|\psi(t)\rangle\langle\psi(t)|\} \\
&= \sum_{m=-v_0}^{v_n-v_0}\sum_{m'=-v_0}^{v_n-v_0} P^m(t)P^{m'}(t)^*|v_0+m\rangle\langle v_0+m'|\delta_{m,m'} \\
&= \sum_{m=-v_0}^{v_n-n_0} |P^m(t)|^2|v_0+m\rangle\langle v_0+m| \\
&= \sum_{m=-v_0}^{v_n-n_0} \mathcal{P}^m(t)|v_0+m\rangle\langle v_0+m|. \qquad (6)
\end{aligned}
$$

According to the method in the reference [13], the generalized geometric Quantum Speed Limits which represents a generic evolution between an initial stateρ_0 and a final stateρ_τ may be reduced as

$$
\mathcal{G}(\rho_0,\rho_\tau) = \int_0^\tau \sqrt{g(t)}dt, \qquad (7)
$$

since the evolution is unitary in our molecular system. g represents any contractive Riemannian metric, when considering the quantum Fisher information metric and the Wigner-Yanase information metric, respectively, it can be written as

$$g^{QF}(t)=\frac{1}{2\hbar^2}\sum_{m,m'}\frac{(\mathcal{P}^m-\mathcal{P}^{m'})^2}{\mathcal{P}^m+\mathcal{P}^{m'}}\langle v_0+m|\triangle\hat{H}|v_0+m'\rangle\langle v_0+m'|\triangle\hat{H}|v_0+m\rangle, \tag{8}$$

and

$$g^{WY}(t)=\frac{1}{\hbar^2}\sum_{m,m'}(\sqrt{\mathcal{P}^m}-\sqrt{\mathcal{P}^{m'}})^2\langle v_0+m|\triangle\hat{H}|v_0+m'\rangle\langle v_0+m'|\triangle\hat{H}|v_0+m\rangle, \tag{9}$$

in which $\triangle\hat{H}=\hat{H}-\langle\hat{H}\rangle$ and $\mathcal{P}^m$ is the eigenvalues of the evolved state ρ_t. The relative difference is defined as

$$\delta=\frac{\mathcal{G}(\rho_0,\rho_\tau)-\mathcal{L}(\rho_0,\rho_\tau)}{\mathcal{L}(\rho_0,\rho_\tau)}, \tag{10}$$

which quantifies how much the dynamics evolution differ from a geodesic with respect to the considered metric. The more smaller quantity δ is, the tighter geometric QSL will be. $\mathcal{L}(\rho_0,\rho_\tau)$ is defined as the geodesic distance between the initial state ρ_0 and the final state ρ_τ, its analytic expressions are known only related to the quantum Fisher information metric [25] and the Wigner-Yanase information metric [26]

$$\mathcal{L}^{QF}(\rho_0,\rho_\tau)=arccos\left(Tr[\sqrt{\sqrt{\rho_0}\rho_\tau\sqrt{\rho_0}}]\right), \tag{11}$$

and

$$\mathcal{L}^{WY}(\rho_0,\rho_\tau)=arccos(Tr[\sqrt{\rho_0}\sqrt{\rho_\tau}]). \tag{12}$$

3 Results and disscussions

We here take the triatomic molecules HCN and DCN as concrete examples since the two molecules have been successfully applied to study the vibrational excitation control and dynamical entanglement [19, 20, 22]. The parameters of HCN and DCN molecules are given in our previous work [27].

According to the Sec. 2, the dynamical evolution from the initial state $\rho_0=|\psi(0)\rangle\langle\psi(0)|$ to the final state ρ_τ need to be investigated, hence the various initial states $v_0=3,6,9,12$ are considered in our current work. The relative differences δ for the various initial states in HCN and DCN molecules are given in Figs. 1 and 2. From these two figures, we can see the relative differences δ of the quantum Fisher information metric are both smaller than the one of the Wigner-Yanase information metric for HCN and DCN molecules, which means the former metric is tighter than the latter one, that is to say, the geometric

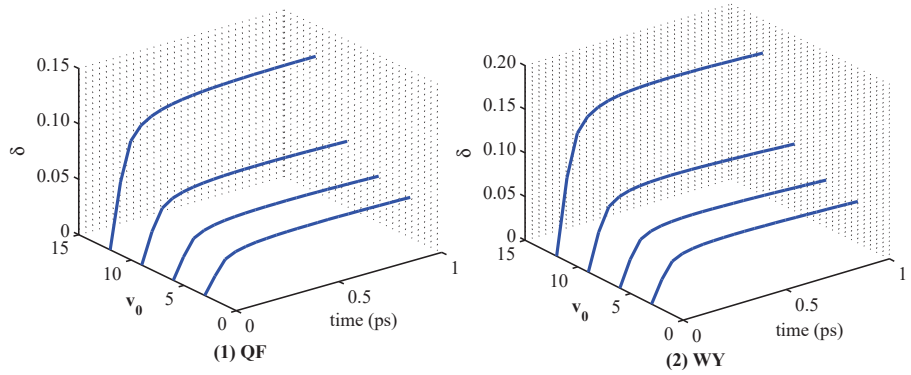

Figure 1: The relative differences δ corresponding to the quantum Fisher information metric (QF) and the Wigner-Yanase information metric (WY) for the initial states $v_0 = 3,6,9,12$ in HCN.

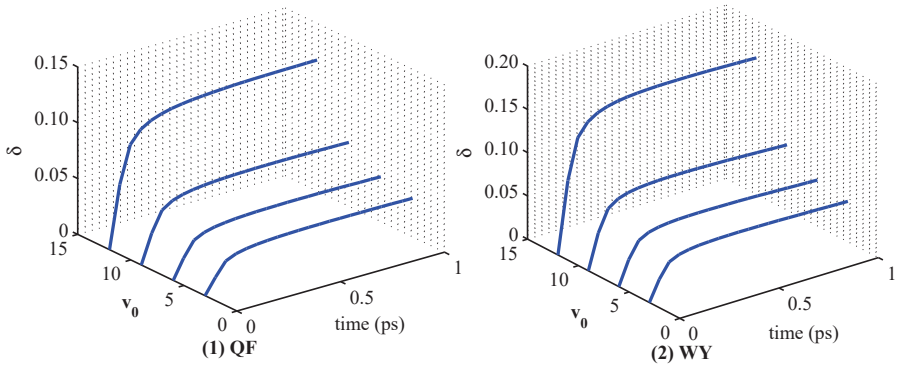

Figure 2: The relative differences δ corresponding to the quantum Fisher information metric (QF) and the Wigner-Yanase information metric (WY) for the initial states $v_0 = 3,6,9,12$ in DCN.

QSL based on the quantum Fisher information metric is more suitable to describe the molecular dynamical evolution. However, with the increase of the vibrational state, the relative difference δ become larger indicates that the general geometric QSL metric is no longer adequate for studying the higher vibrational dynamical evolution. We can also find the relative difference δ for the DCN molecule are smaller than the one for the HCN molecule, which manifest the different molecules can affect the accuracy of the QSL metric, we need minimizing the relative difference over different metrics in order to give the tightest metric QSL for different molecules.

4 Conculsions

The quantum speed limit metrics for molecules have been researched successfully using the algebraic approach. The geometric QSL corresponding to the quantum Fisher information metric is more suitable to describe the dynamical evolution in molecules. The QSL metric is not only related to the initial evolution states but also to the molecule itself. In the following work, the approach can be extended to study the affect of the initial mixed states for the QSL metric, and the quantum limit speed time for a given dynamical evolution in realistic molecules can also be studied.

Acknowledgments. This work is supported by the National Natural Science Foundation of China under Grant No.11147019 and No.11504135.

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