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Fidelity and Mutual Entropy in Mixed States for Fermi-resonance Coupling Vibrations of CS_2

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The dynamics of four fidelities is studied for mixed coherent states and mixed squeezed states of Fermi-resonance coupling vibrations in molecule CS_2. It is demonstrated that those fidelities are dominant-positively correlated with each other, one of which by Wang *et al.* (Phys. Lett. A **373**, 58 (2008)) is the most striking in dominant anti-correlation with quantum mutual entropy. That is useful for molecular quantum computing and quantum information.

Key words: Fidelity, Quantum mutual entropy, Vibrational analysis

I. INTRODUCTION

Fidelity is an important quantity that is extensively applied to quantum computation and quantum information. For molecular quantum computing, extremely high quantum gate fidelity can be achieved for a qubit system based on vibrational eigenstates with increase of anharmonicity parameter in diatomic molecules [1], and the maximal fidelity can be realized with quantum computational gates on the energy levels in a molecular ion [2] and a polyatomic molecule [3]. Much recently, novel fidelities [4–6] have been proposed. For two mixed thermal states the fidelity introduced in Ref.[4] is connected to the operator fidelity [7] for two unitary evolution operators by the Wick rotation. The static difference among those fidelities has been analyzed for mixed states of qudits [4]. Actually, quantum information process needs the time evolution of fidelity and other quantities. The degree of dynamical difference among those fidelities for a common initial state is critically important in the more effective realization of quantum information process and some other tasks. In the present work we study the dynamical difference among those fidelities for the bending and stretching modes based on the experimental spectra of molecule CS_2 [8], where the bend and the stretch are coupled with 2:1 Fermi resonance. It should be pointed out that Fermi resonances are nowadays playing a remarkable role in the understanding of complex experimental situations [8–13]. Two kinds of useful initial states that are mixed states of coherent states and squeezed states on each mode are used to examine the dynamics of fidelity. The dynamical correlation between fidelity and

quantum mutual entropy is discussed as well.

II. HAMILTONIAN

We use molecule CS_2 as our model. Measuring the stretching and bending vibrational spectra of CS_2 with high resolutions, Pique and coworkers have proposed an effective Hamiltonian for the understanding of the major bands in the overtone region with a considerable insight into the nature of the vibrations. The Hamiltonian reads [8]

$$H = H_0(v_1, v_2) + \frac{1}{\sqrt{2}}k_{122}(a_1^\dagger a_2 a_2 + a_1 a_2^\dagger a_2^\dagger) \quad (1)$$

$$H_0(v_1, v_2) = \omega_1'\left(v_1 + \frac{1}{2}\right) + \omega_2'(v_2 + 1) + X_{11}\left(v_1 + \frac{1}{2}\right)^2 + X_{22}(v_2 + 1)^2 + X_{12}\left(v_1 + \frac{1}{2}\right) + (v_2 + 1)Y_{222}(v_2 + 1)^3 \quad (2)$$

where $v_{1(2)}$ is quantum number on the stretch (bend), indexes 1 and 2 stand for the degree of freedom on stretching and bending mode, respectively. a_i and $a_i^\dagger$ (i=1, 2) are the annihilation and creation operators on mode i. ω_1', ω_2', X_{11}, X_{22}, X_{12}, Y_{222}, and k_{122} have their usual spectroscopic meaning with k_{122} being the Fermi coupling parameter between the stretch and the bend. Fitting highly excited spectra of CS_2 up to 1200 cm^{-1}, Pique and coworkers have presented the optimized parameters [8], where the classical dynamics was studied. Details for spectroscopic Hamiltonian are referred to Refs.[14, 15]. We employ those parameters of CS_2 to investigate quantum dynamics of fidelity and quantum mutual entropy.

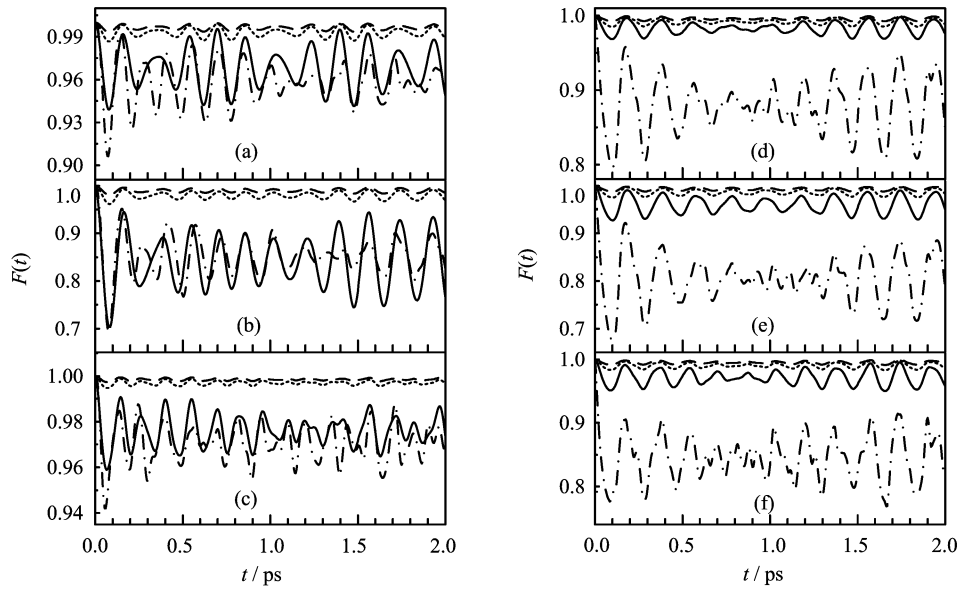*Author to whom correspondence should be addressed. E-mail: xwhou@phy.ccnu.edu.cn

FIG. 1 Four fidelities $F(t)$ (—), $F_1(t)$ (− · −), $F_2(t)$ (− −), and $F_3(t)$ (· · ·) for MCSs (a), (b), (c) and MSSs (d), (e), (f) with parameters $(\overline{v}_1, \overline{v}_2)$ being taken to be (0.5, 0.5), (1.2, 0.5), and (0.5, 1.2), respectively.

III. DYNAMICS OF FIDELITY AND MUTUAL ENTROPY

We are interested in two kinds of initial states to study the time-evolution of fidelity and mutual entropy. The importance of studying both quantities in different initial states is twofold. It may be viewed as a key to the understanding of some of the striking differences between the quantum and classical description of the world. Continuous-variable-type entangled states including squeezed states and coherent states have been widely applied to quantum teleportation [16] and quantum cryptography [17]. So it is important to investigate dynamics of fidelity and mutual entropy for both kinds of states.

The mixed density matrices of initial states of full system is taken to be

$$\rho(0) = \rho_1(0) \otimes \rho_2(0) \tag{3}$$

$$\rho_i(0) = \sum_{v_i=0}^{N_i} P_A(v_i, \overline{v}_i)|v_i\rangle\langle v_i| \tag{4}$$

where $\rho_i(0)$ is the initial density matrix of mode i. The subscript A represent the coherent states C and the squeezed states S on mode i with the coefficients being [18],

$$P_C(v_i, \overline{v}_i) = e^{-\overline{v}_i} \frac{\overline{v}_i^{v_i}}{v_i!} \tag{5}$$

$$P_S(v_i, \overline{v}_i) = \begin{cases} \dfrac{v_i!}{\cosh r} \left[\left\{ \dfrac{v_i}{2} \right\}! \right]^{-2} \left[\dfrac{\tanh r}{2} \right]^{v_i}, & v_i \text{ even} \\ 0, & v_i \text{ odd} \end{cases} \tag{6}$$

where $r = \text{arcsinh}\sqrt{\overline{v}_i}$ and $\overline{v}_i$ is the average quantum

number on mode i, which will be taken as a parameter in what follows. The density matrix of full system evolves in time with the Liouville equation,

$$\dot{\rho}(t) = -i[\hat{H}, \rho(t)] \tag{7}$$

We explore the fidelity dynamics for two density matrices $\rho(0)$ and $\rho(t)$ of interest. The latest defined fidelity is given by [4]

$$F(t) = \frac{|\text{Tr}\,[\rho(0)\rho(t)]|}{\sqrt{\text{Tr}\,[\rho(0)^2]\,\text{Tr}\,[\rho(t)^2]}} \tag{8}$$

The fidelity is also defined as [5]

$$F_1(t) = \text{Tr}\,[\rho(0)\rho(t)] + \sqrt{1 - \text{Tr}\,[\rho(0)^2]} \cdot \\ \sqrt{1 - \text{Tr}\,[\rho(t)^2]} \tag{9}$$

Another fidelity that is essentially the same as $F_1(t)$ is defined by [6]

$$F_2(t) = \frac{1-r}{2} + \frac{1+r}{2}F_1(t) \tag{10}$$

where $r=1/(d-1)$ with d being the dimension of the Hilbert space. The Uhlmann's fidelity is given as [19]

$$F_3(t) = \left[\text{Tr}|\sqrt{\rho(0)}\sqrt{\rho(t)}| \right]^2 \tag{11}$$

Figure 1 shows those four fidelities $F(t)$, $F_1(t)$, $F_2(t)$, and $F_3(t)$ for mixed coherent states (MCSs) and mixed squeezed states (MSSs) with parameters $(\overline{v}_1, \overline{v}_2)$ being, taken to be (0.5, 0.5), (1.2, 0.5), and (0.5, 1.2), respectively. It is observed that these fidelities with
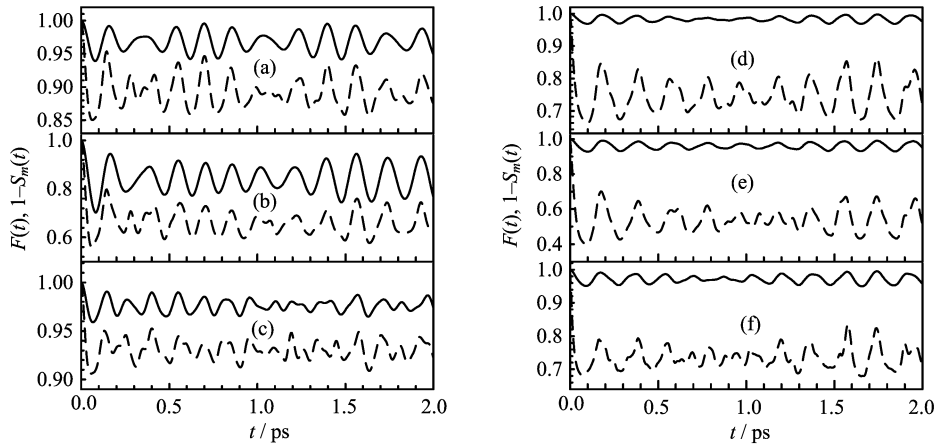
FIG. 2 Fidelity $F(t)$ (solid line) and effective mutual entropy $1-S_m(t)$ (dashed line), for MCSs (a), (b), (c) and MSSs (d), (e), (f) with parameters $(\bar{v}_1, \bar{v}_2)$ being taken to be (0.5, 0.5), (1.2, 0.5), and (0.5, 1.2), respectively.

their oscillation amplitudes obey inequalities, $F(t)$ or $F_3(t) \geq F_1(t) \geq F_2(t)$ in the most of evolution time for MCSs and $F_3(t) \geq F(t) \geq F_1(t) \geq F_2(t)$ for MSSs, so do their decreasing rates in the early-time evolution. Two different correlations are found in Fig.1. The first type of correlation is a case where both quantities rise and lower together, and the second type of correlation is a case where they are anti-correlated, that is, one quantity increases with time while another decreases or vice versa. It is easy to see that $F_1(t)$ and $F_2(t)$ are positively correlated, as shown in their definitions, which makes it possible to discuss only the correlations of both $F_1(t)$ and $F_3(t)$ with $F(t)$. In order to determine quantitatively correlation behaviors of both quantities, we can introduce a correlation parameter since both are dimensionless, which is defined by

$$p(t_j) = \frac{\Delta F_i(t_j)}{\Delta F(t_j)} \tag{12}$$

$$\Delta F_i(t_j) = F_i(t_j) - F_i(t_{j-1}), \quad (i = 1 \text{ and } 3) \tag{13}$$

$$\Delta F(t_j) = F(t_j) - F(t_{j-1}) \tag{14}$$

the smaller of both changes is substituted in the numerator, and j is for the index of time evolution. When $p(t_j)$ is positive, $F_i(t_j)$ and $F(t_j)$ are positively correlated, whereas when it is negative they are anti-correlated. The correlation parameter $p(t_j)$ for $F_1(t)$ and $F(t)$ is always positive while positive or negative $p(t_j)$ for $F_3(t)$ and $F(t)$ appears in an irregular manner. However, the positive correlation between $F_3(t)$ and $F(t)$ is dominant. That demonstrates that four fidelities are dominant-positively correlated with each other. Thus we would like to discuss the correlation of fidelity $F(t)$ with quantum mutual entropy.

The quantum mutual entropy is defined by [20]

$$S_m(t) = S_1(t) + S_2(t) - S(t) \tag{15}$$

$$S_i(t) = -\text{Tr}[\rho_i(t) \ln \rho_i(t)] \tag{16}$$

$$\rho_{1(2)} = \text{Tr}_{2(1)}\rho(t) \tag{17}$$

where $S_i(t)$ is the reduced von Neumann entropy, and $S(t)$ is the von Neumann entropy of the full system, which is constant for the Hamiltonian evolution governed by Eq.(1). It should be mentioned that the entropy for various pure states in other models has been studied in Ref.[21–23]. For a pure state one has $S_1(t) = S_2(t)$ and $S_m(t) = 0$ [20].

Figure 2 shows an effective mutual entropy, $1-S_m(t)$, and fidelity $F(t)$ for the same states as in Fig.1, for the convenience of comparison. It is noted that for given parameters in MCSs both quantities are dominantly positive correlation. The simulated correlation parameter $p(t_j)$ for $1-S_m(t)$ and $F(t)$ becomes positive or negative in an irregular way with the time evolution. However, the area $\int p(t)\mathrm{d}t$ we calculated is always positive. That indicates that $F(t)$ and $1-S_m(t)$ are indeed dominantly positive correlation, implying that $F(t)$ and $S_m(t)$ are dominantly anti-correlated. The correlated behavior for MSSs is similar. For given parameters in initial states the area for MCSs is larger than that for MSSs, showing that MCSs has an advantage over MSSs. It should be pointed out that other three fidelities are also dominantly anti-correlated with the mutual entropy. However, such a correlation between $F(t)$ and $S_m(t)$ is the most striking.

IV. CONCLUSION

In summary, we have compared the dynamics of four fidelities for MCSs and MSSs in the stretch and bend vibrations in molecule CS$_2$. It is shown that those fidelities are dominant-positively correlated. Furthermore, it is demonstrated that fidelity $F(t)$ is the most distinct in dominant anti-correlation with the quantum mutual entropy. It should be remarked that the above conclusion can be applied to other Fermi resonance systems.

Considering the correlated behavior with a large oscillatory amplitude and other properties [4, 24], we believe that the fidelity ($F(t)$) by Wang and coworkers [4] and the Uhlmann's fidelity ($F_3(t)$) are useful in quantum information. More investigations are, however, needed to judge which is better.

It is desirable to use both fidelities for molecular quantum computing. It is possible to study entanglement for mixed states, and results will be discussed elsewhere.

V. ACKNOWLEDGMENT

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