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Fidelity susceptibility for SU(2)-invariant states

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Abstract

We study the fidelity susceptibility of two SU(2)-invariant reduced density matrices. Due to the commuting property of these matrices, analytical results for reduced fidelity susceptibility are obtained and can be applied to study quantum phase transitions in SU(2)-invariant systems. As an example, we analyze the quantum criticality of the spin-1 bilinear-biquadratic model via the fidelity approach.

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1. Introduction

In 1984, Peres introduced the concept of fidelity to characterize quantum system responses to a perturbation [1]. It is of fundamental importance when studying quantum dynamics and has been applied to characterize two important phenomena in condensed matter theory, quantum chaos and quantum phase transitions (QPTs) [2–8]. It also became a useful concept in quantum information theory [9], and has been used in the study of quantum entanglement theory [10], quantum teleportation [11], transformation of unknown states [12], etc.

As an indicator of QPTs, various kinds of fidelity have been used in investigating the quantum phase transition point, such as Loschmidt echo [3], ground-state fidelity [13], the fidelity of the first excited state [14], operator fidelity [15, 16], reduced fidelity [17, 18], etc. The fidelity susceptibility (FS) [5], as the leading term of the fidelity, can be conveniently used to detect QPTs for its independence of the concrete values of small perturbations. As we consider QPTs, the ground-state FS is a natural choice for the present study. Ground-state fidelity was studied in different physical systems such as the Bose–Hubbard model [19], Bose–Einstein condensate [20] and spin chains [21].

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Let us briefly introduce quantum fidelity and fidelity susceptibility. For pure states, fidelity is the absolute value of an overlap of two wavefunctions. One important case is the fidelity between the ground state $|\psi_0(x)\rangle$ of the Hamiltonian $H(x)$ and a slightly different one $|\psi_0(x + \delta)\rangle$:

$$F = |\langle \psi_0(x) | \psi_0(x + \delta) \rangle|, \quad (1)$$

where δ is a small deviation. Substituting the expansion

$$|\psi(x + \delta)\rangle = |\psi(x)\rangle + \delta|\dot{\psi}(x)\rangle + \delta^2/2|\ddot{\psi}(x)\rangle + O(\delta^3) \quad (2)$$

into the above equation leads to

$$\begin{aligned} F &= 1 + \frac{\delta^2}{4}(\langle \psi_0 | \ddot{\psi}_0 \rangle + \langle \ddot{\psi}_0 | \psi_0 \rangle + 2|\langle \psi_0 | \dot{\psi}_0 \rangle|^2) \\ &= 1 - \frac{\delta^2}{2}(\langle \dot{\psi}_0 | \dot{\psi}_0 \rangle - |\langle \psi_0 | \dot{\psi}_0 \rangle|^2). \end{aligned} \quad (3)$$

One may further define the FS as [5]

$$\begin{aligned} \chi_F &= \lim_{\delta \rightarrow 0} \frac{2(1 - F)}{\delta^2} = \langle \dot{\psi}_0 | \dot{\psi}_0 \rangle - |\langle \psi_0 | \dot{\psi}_0 \rangle|^2 \\ &= \sum_{n \neq 0} |\langle \psi_n | \dot{\psi}_0 \rangle|^2. \end{aligned} \quad (4)$$

So, the FS is explicitly written out in terms of eigenstates. However, for a mixed-state case, the corresponding fidelity and FS are relatively difficult to be achieved. One can use Uhlmann's fidelity [22]

$$F = \text{tr} \sqrt{\varrho^{1/2} \tilde{\varrho} \varrho^{1/2}} \quad (5)$$

for two mixed states ϱ and $\tilde{\varrho}$ and the corresponding FS can also be defined as above. In what follows, we analyze the fidelity of SU(2)-invariant mixed states by this definition.

For a many-body quantum state, by tracing out other degrees of freedom but two particles, we have a two-particle reduced-density matrix which is generally a mixed state. Fidelity between reduced density matrices is called reduced fidelity [17]. For some interesting physical models such as the spin-1 bilinear-biquadratic model [23–26] and spin-half frustrated model, the reduced-density matrix displays an SU(2) symmetry. In this paper, we will study the fidelity of the SU(2)-invariant state. The symmetry in this state greatly facilitates our study of fidelity, and analytical results are obtained for the fidelity susceptibility. We also give an application of the results to study the quantum phase transition in the bilinear-biquadratic model.

2. SU(2)-invariant states and FS

Before proceeding, we make it clear that if a multi-spin state ρ displays a global SU(2) symmetry ($[\rho, \mathbf{J}] = 0$), the two-spin reduced-density matrix also has an SU(2) symmetry ($[\rho_{12}, \mathbf{j}_1 + \mathbf{j}_2] = 0$), where $\mathbf{J} = \mathbf{j}_1 + \cdots + \mathbf{j}_N$ is the collecting spin operator. The proof is straightforward. The commutator $[\rho, \mathbf{J}] = 0$ means that

$$[\rho, \mathbf{j}_1 + \mathbf{j}_2] = [\mathbf{j}_3 + \cdots + \mathbf{j}_N, \rho]. \quad (6)$$

After tracing out the degree of freedom of spins $3 \rightarrow N$, we have

$$[\rho_{12}, \mathbf{j}_1 + \mathbf{j}_2] = \text{Tr}_{3 \rightarrow N} [\mathbf{j}_3 + \cdots + \mathbf{j}_N, \rho] = 0. \quad (7)$$

An SU(2)-invariant state of two spins j_1 and j_2 can be written in the general form

$$\rho = \sum_{J=|j_1-j_2|}^{j_1+j_2} \frac{\alpha_J}{2J+1} P_J, \tag{8}$$

where $\alpha_J \geq 0$, $\sum_J \alpha_J = 1$ and P_J is the projector of the spin- J subspace. Obviously, the density operator has eigenvalues $\alpha_J/(2J+1)$ with degeneracy $2J+1$.

One key observation from the above equation is that two different SU(2)-invariant density matrices ρ and $\tilde{\rho}$ commute with each other. Thus, they can be diagonalized simultaneously, and the fidelity between them is given by

$$F = \sum_{k=1}^{j_1 j_2} \sqrt{\lambda_k \tilde{\lambda}_k}, \tag{9}$$

where λ_k 's and $\tilde{\lambda}_k$'s are the eigenvalues of ρ and $\tilde{\rho}$, respectively. Since zero eigenvalues have no contribution to F , we only need to consider the nonzero ones. In the following, the subscript k in \sum_k only denotes nonzero eigenvalues of ρ .

Now we calculate the fidelity of two slightly different density matrices $\rho(x)$ and $\rho(x+\delta)$ as a function of parameter x , where δ is a small change of x . It is noted that, for a small change δ , we have

$$\lambda_k(x+\delta) \simeq \lambda_k + (\partial_x \lambda_k)\delta + (\partial_x^2 \lambda_k)\delta^2/2 + O(\delta^3). \tag{10}$$

Substituting this expression into equation (9) leads to the fidelity given by

$$F = 1 - \frac{\delta^2}{2} \sum_i \frac{(\partial_x \lambda_k)^2}{4\lambda_k}. \tag{11}$$

In deriving the above equation, we have used $\sum_i \lambda_i \equiv 1$ and $\sum_i \partial_x \lambda_i = \sum_i \partial_x^2 \lambda_i = 0$. Therefore, according to the relation between the fidelity and FS $F = 1 - \chi \delta^2/2$ [5], the FS χ_F corresponding to the matrix ρ is obtained as

$$\chi_F = \sum_k \frac{(\partial_x \lambda_k)^2}{4\lambda_k}. \tag{12}$$

This expression of fidelity susceptibility is valid for any commuting density matrices. It depends on nonzero eigenvalues of ρ and their first-order derivatives.

Applying equation (12) into the SU(2)-invariant state ρ (8), one obtains the FS for ρ as

$$\chi_F = \sum_{J=j_2-j_1}^{j_1+j_2} \frac{(\partial_x \alpha_J)^2}{4\alpha_J}, \tag{13}$$

where we assumed $j_2 > j_1$ without loss of generality. Now, we consider the following cases of $j_1 = 1/2$ and $j_2 \geq 1/2$. As $\alpha_{j_2-1/2} + \alpha_{j_2+1/2} = 1$, equation (13) reduces to

$$\chi_F = \frac{(\partial_x \alpha_{j_2-1/2})^2}{4\alpha_{j_2-1/2}(1 - \alpha_{j_2-1/2})}. \tag{14}$$

Parameter $\alpha_{j_2-1/2}$ can be written in terms of the expectation of the Heisenberg interaction on ρ , $(\mathbf{j}_1 \cdot \mathbf{j}_2)$, i.e. [27]

$$\alpha_{j_2-1/2} = \frac{1}{2j_2+1} (j_2 - 2\langle \mathbf{j}_1 \cdot \mathbf{j}_2 \rangle). \tag{15}$$

Thus, equation (14) can be reexpressed in the following form:

$$\chi_F = \frac{(\partial_x \langle \mathbf{j}_1 \cdot \mathbf{j}_2 \rangle)^2}{(j_2 - 2\langle \mathbf{j}_1 \cdot \mathbf{j}_2 \rangle)(j_2 + 1 + 2\langle \mathbf{j}_1 \cdot \mathbf{j}_2 \rangle)}. \tag{16}$$

We see that for the SU(2)-invariant state, the FS is completely determined by the expectation value of the Heisenberg interaction and its first-order derivative. If we consider the case of two qubits, then the above equation reduces to

$$\chi_F = \frac{4(\partial_x \langle \mathbf{j}_1 \cdot \mathbf{j}_2 \rangle)^2}{(1 - 4\langle \mathbf{j}_1 \cdot \mathbf{j}_2 \rangle)(3 + 4\langle \mathbf{j}_1 \cdot \mathbf{j}_2 \rangle)}, \quad (17)$$

which is just the FS obtained in [28] via a different approach.

Now, we study the case of two qutrits, i.e. two spin ones. From equation (8), one has

$$\begin{aligned} \alpha_0 &= \langle P_0 \rangle = \langle P_{12} \rangle, \\ \alpha_1 &= \langle P_1 \rangle = \frac{1}{2}(1 - \langle S_{12} \rangle), \\ \alpha_2 &= \langle P_2 \rangle = \frac{1}{2}(1 - 2\langle P_{12} \rangle + \langle S_{12} \rangle), \end{aligned} \quad (18)$$

where

$$\begin{aligned} P_{12} &= \frac{1}{3}[(\mathbf{j}_1 \cdot \mathbf{j}_2)^2 - 1], \\ S_{12} &= \mathbf{j}_1 \cdot \mathbf{j}_2 + (\mathbf{j}_1 \cdot \mathbf{j}_2)^2 - 1 \end{aligned} \quad (19)$$

are the singlet projection operator and swap operator, respectively. Substituting equations (18) and (19) into equation (13) leads to the FS for two qutrits:

$$\chi_F = \frac{1}{4} \left[\frac{(\partial_x \langle P_{12} \rangle)^2}{\langle P_{12} \rangle} + \frac{(\partial_x \langle S_{12} \rangle)^2}{2(1 - \langle S_{12} \rangle)} + \frac{(\partial_x \langle S_{12} \rangle - 2\partial_x \langle P_{12} \rangle)^2}{2(1 - 2\langle P_{12} \rangle + \langle S_{12} \rangle)} \right]. \quad (20)$$

The FS is determined by two expectation values $\langle P_{12} \rangle$ and $\langle S_{12} \rangle$ and their first-order derivatives. Below, we will apply this formula to the study of the bilinear-biquadratic model.

3. Applications to spin-1 systems

Spin Heisenberg chains attract more attention since Haldane predicted that the one-dimensional chain has a spin gap for integer spins [29]. In these studies, the bilinear-biquadratic model has played an important role [23–26]. The corresponding Hamiltonian is given by

$$\begin{aligned} H_{BB} &= \sum_{i=1}^N \cos \theta (\mathbf{j}_i \cdot \mathbf{j}_{i+1}) + \sin \theta (\mathbf{j}_i \cdot \mathbf{j}_{i+1})^2, \\ &= \sum_{i=1}^N [\cos \theta S_{i,i+1} + 3(\sin \theta - \cos \theta) P_{i,i+1}] + N \sin \theta. \end{aligned} \quad (21)$$

In deriving the last equality, we have used equation (19). Here, \mathbf{j}_i denotes the spin-1 operator at site i , and we have assumed the periodic boundary conditions. The Hamiltonian exhibits an SU(2) symmetry and displays very rich quantum phase diagrams [30]. One can also use other boundary conditions such as the open boundary condition, for which the reduced density matrix still has the SU(2) symmetry.

From the Hellmann–Feymann theorem for the ground state, one can easily find that

$$\begin{aligned} \langle P_{12} \rangle &= \frac{1}{3}(\sin \theta e_0 + \cos \theta e'_0 - 1), \\ \langle S_{12} \rangle &= (\cos \theta + \sin \theta) e_0 + (\cos \theta - \sin \theta) e'_0 - 1 \end{aligned} \quad (22)$$

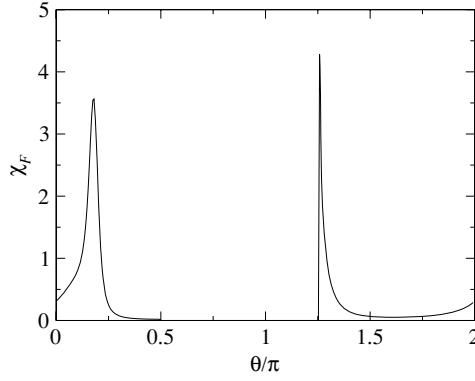


Figure 1. Ground-state fidelity susceptibility as a function of θ/π in the bilinear-biquadratic model.

and their first-order derivatives

$$\begin{aligned}\langle P_{12} \rangle' &= \frac{\cos \theta}{3} (e_0 + e_0''), \\ \langle S_{12} \rangle' &= (\cos \theta - \sin \theta) (e_0 + e_0''), \\ \langle S_{12} \rangle' - 2 \langle P_{12} \rangle' &= \left(\frac{\cos \theta}{3} - \sin \theta \right) (e_0 + e_0'').\end{aligned}\quad (23)$$

Here, e_0 denotes the ground-state energy per site. Substituting the above two equations into (20), one obtains the FS in terms of e_0 , e_0' and e_0'' as follows:

$$\chi_F = \frac{(e_0 + e_0'')^2}{4} \left[\frac{\cos^2 \theta}{3(\sin \theta e_0 + \cos \theta e_0' - 1)} + \frac{(\cos \theta - \sin \theta)^2}{2[2 - (\cos \theta + \sin \theta)e_0 - (\cos \theta - \sin \theta)e_0']} \right. \\ \left. + \frac{(\cos \theta - 3 \sin \theta)^2}{6[2 + (3 \cos \theta + \sin \theta)e_0 + (\cos \theta - 3 \sin \theta)e_0']} \right]. \quad (24)$$

One key observation is that the numerators of the above two expressions happen to be proportional to $(e_0 + e_0'')^2$. Then, we infer that if the second derivative of the ground-state energy is singular at the critical point, the FS is singular too. On the other hand, it is known that the divergence of the second derivative of the ground-state energy reflects the second-order QPTs of the system, which is shown in [13] explicitly as

$$\partial_\alpha^2 e_0 = \sum_{n \neq 0}^N \frac{2 |\langle \Psi_n | \partial_\alpha H | \Psi_n \rangle|^2}{N(E_0 - E_n)},$$

where $|\Psi_n\rangle$ is the eigenvector corresponding to the eigenvalue E_n . It shows that the vanishing energy gap in the thermodynamic limit can lead to the singularity of the second derivative of the ground-state energy. Therefore, the two-spin FSs can exactly reflect the second-order QPTs of the global system in this model.

We use the exact-diagonalization method to calculate the ground-state energy and then numerical results of FS are obtained from equation (24). In figure 1, we plot the FS as a function of θ for a sample of 12 spins. We observe a sharp decrease of the FS around $\theta = \pi/4$, which separates the Haldane phase ($-\pi/4 < \theta < \pi/4$) and the trimerized phase ($\pi/4 < \theta < \pi/2$). This may imply that a QPT occurs. For $\pi/2 < \theta < 5\pi/4$, the ground state is ferromagnetic and degenerate. In this range, the FS is zero. However, at $\theta = 7\pi/4$,

corresponding to a QPT point separating the dimerized phase ($5\pi/4 < \theta < 7\pi/4$) and Haldane phase, one cannot find any anomalous behaviors of the FS.

4. Conclusions

We have studied the FS in SU(2)-invariant states and have obtained an exact analytical expression of the FS for any spins j_1 and j_2 . This implies that the results are applicable to equal-spin as well as mixed-spin systems. Furthermore, one can use the FS to study the properties of SU(2)-invariant physical systems in a finite-temperature thermal state. As an application, we have studied relations between the FS and QPTs in the bilinear-biquadratic model. For this model, one can infer that the two-spin FS can exactly reflect the second-order QPTs of the global system.

Here, we restrict ourselves to study SU(2)-invariant states of two spins, after tracing out other spins of a many-body state. One can also use quantum entanglement as an indicator of QPTs. As stated in [19], one main advantage of fidelity lies in the fact that it does not require any *a priori* knowledge of the correlations driving the QPT. One challenge for further investigation is to study the N -spin ($N \geq 3$) SU(2)-invariant reduced density matrix. The present approach can be generalized to quantum states with other certain symmetries such as SU(3) symmetry, and analytical results of fidelity are expected.

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