Operator fidelity approach to the quantum phase transition of the spin-1/2 XX chain with three-spin interaction and the (1/2,1) XXZ mixed-spin chain

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Abstract. We make use of the operator fidelity and its susceptibility to study the quantum phase transition (QPT) of the spin-1/2 XX spin chain with three-spin interaction. The analytical results of operator fidelity and the susceptibility are obtained. From the numerical results one can see that the operator fidelity and its susceptibility present nontrivial behaviors at the critical point. We also consider the (1/2, 1) XXZ mixed-spin chain in which the ground states are degenerate. The operator fidelity approach is still effective to indicate the QPT in this system. We also generally analyze the relation between operator fidelity and QPT.

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1. Introduction

In quantum many-body correlated system, the quantum phase transition (QPT) is an essential phenomenon and attracts widespread attention. The QPT occurs at zero temperature and it is induced purely by quantum fluctuation. Generally, the QPT behaves as the configuration transition of the ground state (GS) driven by perturbations of system parameters. In order to characterize QPTs, an effective method is to use the order parameter and symmetry breaking within the Landau–Ginzburg paradigm [1]. However, the order parameter is model dependent, i.e. there is no general method to find it for a common system. Recently, a concept called fidelity has been introduced to study QPTs, and suggests a universal approach [2]–[4]. The concept of fidelity is borrowed from the field of quantum-information theory, and well describes the overlap between two states with different structural properties. Thus, it does not need a prior knowledge of the order parameter in detecting QPTs. It is a purely Hilbert-space geometrical quantity. The concept of fidelity susceptibility [5, 6] is found to be more convenient than fidelity itself due to its independence of the slightly changed external parameters. By using the fidelity method, the QPTs of many typical systems have been studied, such as the Hubbard model [7], the frustrated Heisenberg chain [8], the Kitaev honeycomb model [9], and the extended Harper model [10]. The intrinsic relation between the GS fidelity (or fidelity susceptibility) and the characterization of a QPT has been unveiled in [11]. It was found that the non-analyticity of the element and its derivative in the density matrix induce the singularity of GS fidelity, which indicates first-order and second-order QPTs. In [12] it was shown that the singularity and scaling behavior of the GS fidelity (or fidelity susceptibility) are directly related to its corresponding derivative of the GS energy, which conventionally characterizes QPTs. Moreover, the fidelity susceptibility is associated with the dynamic structure factor of QPTs and with the specific heat and magnetic susceptibility for thermal phase transitions [13]. The fidelity method is also used to investigate topological QPTs [14]–[16]. The reduced fidelity (or partial-state fidelity) corresponding to the subsystems has also been considered, and has been shown to reflect the QPTs [16]–[20].

In order to improve the fidelity method, Lu et al focus on the operator extensions of fidelity on general grounds [21]. They introduce the concept of operator fidelity (OF) (operator fidelity susceptibility (OFS)), which is closely associated with decoherence. One here notices that finite-time quantum evolutions correspond to unitary operators which themselves belong to a Hilbert space i.e. the Hilbert–Schmidt one. It follows that some of the results obtained in the fidelity approach for quantum states can naturally be generalized to the operator level. Unlike GS fidelity, operator fidelity contains information about all the eigenstates of the Hamiltonian considered. Moreover, when we consider the case of a maximally mixed state, i.e. $\rho = I/d$ (where $d$ is the dimension of the Hilbert space, and $I$ is the identity operator), the operator fidelity will be in the form of the trace of two operators [22]. In this case, the operator fidelity is dependent on the full Hilbert space and not on a certain state. In some typical systems, such as the Ising spin chain under transverse field, it is shown that the operator fidelity can indicate QPTs effectively [21, 22]. However, the approach of the operator fidelity based on the maximally mixed state is only available in certain systems. Thus, when considering QPTs in other systems, one should use the $\rho$-fidelity of the operator, which is a universal method to characterize first-order and second-order QPTs, and we will prove this in section 2.

Now, let us give a brief introduction to the OF and the OFS associated with a state $\rho$, where the state can be a pure state or a mixed state. The $\rho$-fidelity of the operators $X$ and $Y$
is given by
\[ F_\rho(X, Y) := |\langle X, Y \rangle_\rho| = |\text{Tr}(\rho X^\dagger Y)|, \]
for unitaries \( U_1 \) and \( U_2 \), \( F_\rho(U_1, U_2) \leq 1 \). We also give the operational meaning of the above definition as follows: if \( |\Psi_\rho\rangle \in \mathcal{H} \otimes \mathcal{H} \) is a purification of \( \rho = \sum_i p_i |i\rangle \langle i| \) i.e. \( |\Psi_\rho\rangle = \sum_i \sqrt{p_i} |i\rangle \otimes |i\rangle \) then \( \langle X, Y \rangle_\rho = \langle \psi_\rho(X^\dagger \otimes 1)(Y \otimes 1)|\Psi_\rho\rangle \). This type of purification is general, as the quantity is unitarily invariant in any case. The operator scalar product can be seen as a scalar product of suitable quantum states of a bigger system. This simple remark shows that the operator fidelity (1) quantifies the degree of statistical distinguishability between the two states
\[ |\Psi(A)\rangle := (A \otimes 1)|\Psi_\rho\rangle (A = X, Y). \]

When \( X \) and \( Y \) denote unitary transformations the quantity (1) has the interpretation of visibility strength in properly designed interferometric experiments [23].

Now, following the differential-geometric spirit of [24] we consider the operator fidelity (1) between infinitesimally different unitaries. The leading term in the expansion of (1) will define a quadratic form over the tangent space of the manifold \( \mathcal{U}(\mathcal{H}) \). For full rank \( \rho \) that quadratic form is a metric. The following proposition shows that and its proof is just a direct calculation analogous to the one performed at the state-space level [24].

Let \( \{U_\lambda\} \subset \mathcal{U}(\mathcal{H}) \) be a smooth family of unitaries over \( \mathcal{H} \) parameterized by elements \( \lambda \) of a manifold \( \mathcal{M} \). One finds
\[ F_\rho(U_\lambda, U_{\lambda+\delta\lambda}) = 1 - \chi_\rho(\lambda)\delta\lambda^2/2, \]
where, if \( U' = \partial U/\partial \lambda \), one has
\[ \chi_\rho(\lambda) := \langle U', U' \rangle_\rho - |\langle U', U \rangle_\rho|^2. \]

The quantity above will be referred to as OFS.

In this paper, we will analyze the relation between operator fidelity and the QPT from the viewpoint of the singularity of ground energy and its derivative. We will anatomize the singular behavior of the components in the operator fidelity, i.e. the fidelities between the GSs and the excited states. From the analysis, we will find that the operator fidelity corresponding to a proper state is effective to detect the first-order QPT and second-order QPT; however, the Loschmidt echo corresponding to GS cannot indicate the first-order QPT. We make use of the operator fidelity to study the spin-1/2 XX chain with three-spin interaction, which is an important model with second-order QPT and can be solved exactly. However, in previous studies about fidelity and QPTs, this model is not considered. In our paper, the critical properties of this model can be reflected by the dynamical behaviors of the operator fidelity, which is a novel way of using operator fidelity to detect QPT. We also consider another system, the anisotropic \((1/2, 1)\) mixed-spin chain, in which the first-order QPT happens at the isotropic point. Especially, the GSs of this system are degenerate, which makes the GS fidelity and Loschmidt echo disabled. We will show that the operator fidelity is still effective to detect QPT in this system.

The paper is organized as follows: in section 2, we present a general analysis of the relation between operator fidelity and QPTs. In section 3, we use the operator fidelity to study the QPT in isotropic spin-1/2 XX chain with three-spin interaction. The dynamical behaviors of operator
fidelity will be considered, as the quantum criticality can greatly affect the dynamical behavior. Furthermore, we will show that the OFS can effectively indicate a critical point. In section 4, we will study the operator fidelity and its susceptibility in the anisotropic (1/2, 1) mixed-spin chain. Finally, the conclusion will be given.

2. The relation between operator fidelity and QPT

Let us start from a general Hamiltonian containing a two-body interaction expressed as [25, 26]

\[ H = \sum_{i \neq j} e_{ij} |\alpha_i\rangle \langle \beta_j| + \sum_{ij \neq \gamma \delta} V_{ij\gamma\delta} |\alpha_i\rangle |\beta_j\rangle |\gamma\rangle |\delta\rangle, \]

where \( i \) and \( j \) enumerate \( N \) particles and \( \{|\alpha_i\rangle\} \) is a basis for the Hilbert space. For the non-degenerate GS \(|\psi\rangle\), its GS energy is \( E_0 = \langle \psi | H | \psi \rangle \), and the element of the corresponding two-particle reduced density matrix is \( \rho_{ij} = \langle \psi | \alpha_i \beta_j \rangle \langle \gamma \delta | \psi \rangle \). Thus, the relation between energy and reduced density matrix is \( E_0 = \sum_{ij} Tr[U(\delta \lambda)(U(\lambda))^\dagger \rho_{ij}] \), where \( U_{ij\gamma\delta}(\lambda) = e_{ij} \delta_{\alpha\gamma} \delta_{\beta\delta} / N + V_{ij\gamma\delta} \) with \( N \) the number of particles that particle \( i \) interacts with, and \( \delta^{ij}_{\alpha\beta} \) the Kronecker symbols on particle \( j \). Then using the Feynman–Hellman theorem, the derivatives of energy per particle \( (e_0 \equiv E_0 / N) \) are obtained as

\[ \partial_\lambda e_0 = \frac{1}{N} \sum_{ij} Tr[(\partial_\lambda U(\delta \lambda))(U(\delta \lambda))^\dagger \rho_{ij}], \]

\[ \partial_\lambda^2 e_0 = \frac{1}{N} \sum_{ij} \{Tr[(\partial_\lambda^2 U(\delta \lambda))(U(\delta \lambda))^\dagger \rho_{ij}] + Tr[(\partial_\lambda U(\delta \lambda))(\partial_\lambda \rho_{ij})]\}, \]

where it follows from equation (6) that \( \sum_{ij} Tr[U(\delta \lambda)(\partial_\lambda \rho_{ij})] = 0 \). As is known, according to the classical definition of phase transitions given in terms of the free energy [27], in the limit of \( T = 0 \), a first-order QPT (second-order QPT) is characterized by a non-analyticity in the first (second) derivative of the GS energy. Therefore, if \( U(\delta \lambda) \) is a smooth function of the Hamiltonian parameter \( \lambda \), the origin of first-order QPTs is due to the discontinuity of one or more of the \( \rho_{ij} \) elements at the critical point according to equation (6), whereas, if \( \rho_{ij} \) is finite at the critical point, the origin of second-order QPTs is the fact that one or more of the \( \partial_\lambda \rho_{ij} \) diverge at the critical point. These results easily generalize to the case of a Hamiltonian containing \( n \)-body terms [25].

In [11], the researcher gives a general discussion about the relation between GS fidelity and the QPT. The fidelity \( F(\lambda, \delta) = |\langle \Psi_0(\lambda + \delta \lambda) | \Psi_0(\lambda) \rangle| \) can be expanded as

\[ F(\lambda, \delta) = 1 - \frac{\langle \delta \lambda \rangle^2}{4} \langle \partial \rho_0 \partial \rho_0 \rangle \langle \partial_\lambda \partial_\lambda \delta \lambda \rangle + O[\langle \delta \lambda \rangle^4], \]

where \( \rho_0 = |\Psi_0(\lambda)\rangle \langle \Psi_0(\lambda)\rangle \). Since the matrix elements of the reduce density matrix \( \rho_{ij} \) are linear function of those of \( \rho_0 \), the non-analyticity of the \( \rho_{ij} (\partial_\lambda \rho_{ij}) \) can be reflected by \( \partial \rho_0 / \partial \lambda \). Namely, the GS fidelity can indicate the first-order QPT and second-order QPT and also some higher order QPTs [11].

When we make use of the operator fidelity to characterize QPT, generally the first step is to choose a Hamiltonian \( H' = H(\lambda + \delta \lambda) \), which is slightly different from \( H(\lambda) \), then we choose the time evolution operators \( U_1 = \exp(-iH') \), \( U_2 = \exp(-iH) \) (let \( \hbar = 1 \)) to be two unitary
operators in the definition of operator fidelity (see equation \(1\)). The density matrix \(\rho\) can be expressed in the eigenspace of \(H(\lambda)\) as \(\rho = \sum_{n,m} \rho_{mn} |\Psi_n\rangle \langle \Psi_m|\); however, it is more significant to consider the density \(\rho\) as a mixture of the eigenstates of \(H\), i.e. \(\rho = \sum_n P_n |\Psi_n\rangle \langle \Psi_n|\), with the probability \(\sum_n P_n = 1\), here the non-degenerate states are considered. Then the operator fidelity becomes

\[
\begin{align*}
|\rho U_1^\dagger(t) U_2(t)|^2 &= \left|\sum_{m,n} P_n e^{it(E_m' - E_n)} \left|\langle \Psi_n | \Psi_m\rangle\right|^2 \right| \\
&= |P_0 e^{it(E_0' - E_0)} \left|\langle \Psi_0 | \Psi_0\rangle\right|^2 + P_1 e^{it(E_1' - E_0)} \left|\langle \Psi_1 | \Psi_0\rangle\right|^2 + \cdots + P_1 e^{it(E_1' - E_1)} \left|\langle \Psi_1 | \Psi_1\rangle\right|^2|, \\
\end{align*}
\]

where the states \(|\Psi_m\rangle(|\Psi_m\rangle)\) are the eigenstates corresponding to \(H'(H)\) with the eigenvalues \(E_m'(E_m)\). One can see that the above equation contains the overlaps between all the eigenstates of \(H\) and \(H'\). When we try to investigate the QPT, we can modulate the probability \(P_n\) to preserve the GS and some low-lying excited states as the dominant parts in the \(\rho\). For example, considering the system at a thermal state \(\rho(T)\), one can lower the temperature to capture GS properties. By a similar process we can modulate the probability of the density to make the GS fidelity \(|\langle \Psi_0 | \Psi_0\rangle|^2\) play a key role in equation \((9)\). Now let us give further analyses. In the region beyond the vicinity of the critical point, the states \(|\Psi_m\rangle\) and \(|\Psi_n\rangle\) for \(m \neq n\) can be approximately treated as orthogonal states, namely \(|\langle \Psi_m | \Psi_n\rangle| \approx 0\). Then the operator fidelity nearly equals 1, which is mainly attributed to the term of GS fidelity \(|\langle \Psi_0 | \Psi_0\rangle|\), while the terms \(|\langle \Psi_1 | \Psi_1\rangle|\) and \(|\langle \Psi_2 | \Psi_2\rangle|\) give little contribution. When the system approaches the critical point, GS fidelity decays sharply to zero, which reflects the distinction between the states \(|\Psi_0\rangle\) and \(|\Psi_1\rangle\) which belong to two different phases. Then the operator fidelity will also present a sudden decay at the critical point due to the GS fidelity. However, we should pay attention to the term \(|\langle \Psi_1 | \Psi_0\rangle|^2\) in equation \((9)\). In particular, at the first-order QPT point, the energy level crossing usually happens between GS energy \(E_0\) and the first excited state energy \(E_1\). Thus, the fidelity of \(|\langle \Psi_1 | \Psi_0\rangle|^2\) will jump to 1 at the point, which is contrary to the behavior of GS fidelity \(|\langle \Psi_1 | \Psi_0\rangle|^2\). It means that the sum \(|\langle \Psi_1 | \Psi_0\rangle|^2 + |\langle \Psi_0 | \Psi_0\rangle|^2\) will not present a nontrivial phenomenon at the energy level crossing point. From this point of view, the Loschmidt echo \(|\langle \Psi_0 | U_1^\dagger(t) U_2(t) | \Psi_0\rangle|^2|\) based on the GS may be not effective enough to detect the first-order QPTs. However, the operator fidelity in \((9)\) based on a state \(\rho\) contains different phase terms such as \(e^{it(E_0' - E_0)}\) and \(e^{it(E_1' - E_0)}\), which ensure the effect of GS fidelity from the counteraction of \(|\langle \Psi_1 | \Psi_0\rangle|^2\). Usually, the phases \(e^{it(E_1' - E_0)}\) and \(e^{it(E_1' - E_0)}\) are finitely different, which are due to the following reasons: first, in the study of QPT, we generally consider the systems of finite size to simulate the thermodynamical limit cases, then the energy gap between \(E_0\) and \(E_1\) is finite; second, in order to show the fidelity decay, it is better to consider a finite long time, and the small perturbation \(\delta\) is also finite. Thus, the operator fidelity is available to indicate the first-order QPTs. For the second-order QPTs, the quantum criticality is in terms of the singularity in the second-order derivative of GS energy, which can be captured by the GS fidelity in equation \((9)\). In this case, there is no great counteraction from other terms such as \(|\langle \Psi_1 | \Psi_0\rangle|^2\). It is proved that the GS fidelity susceptibility captures the key element of the GS energy second-order derivative \([12]\); furthermore, fidelity susceptibility might be a more sensitive tool to detect critical points.
Consequently, one can conclude that the operator fidelity is a good measure of distinguishability of two operators, and also a good measure of stability of system. One should note that the operator fidelity approach is operational in cases where level crossing of GSs happens or the GS energy second derivative is divergent. In other cases such as the KT phase transition, it is hard to judge whether the operator fidelity is effective or not. However, in the Heisenberg spin chain with the next-nearest-neighbor interaction, the excited state fidelity can indicate the Berezinskii–Kosterlitz–Thouless (BKT) type quantum phase transition [8], and in the XXZ spin-1/2 chain, the scaling behavior of GS fidelity can reflect KT phase transition [12]. It is heuristic for us to study KT phase transition in these systems by the operator fidelity approach which remains an open problem.

Compared to the GS fidelity, the operator fidelity has some advantages: (i) we can use it to consider the dynamical properties of the system and study the quantum criticality. In a time region that is not very long, the operator fidelity approximately behaves as $1 - K \delta^2 \tau^2$ [28], where the parameter $K$ contains the main parts of the OFS. At the critical point, $K$ is divergent which will make the dynamic behavior of fidelity different from the cases beyond the critical region; (ii) due to the close relation to quantum decoherence, the operator fidelity is applicable in experiments. Moreover, by controlling the evolution time, the singular phenomenon of operator fidelity and its susceptibility can be enlarged, which is good for detecting the critical point; (iii) in systems with degenerate GSs, the operator fidelity is still effective to indicate QPTs (see section 4).

3. The spin chain with three-spin interaction

The system we considered is the isotropic spin-1/2 XX chain with three-spin interaction [29, 30],

$$H = - \sum_{l=-M}^{M} \left[ \sigma^x_l \sigma^x_{l+1} + \sigma^y_l \sigma^y_{l+1} + \frac{\lambda}{2} \left( \sigma^x_{l-1} \sigma^x_l \sigma^y_{l+1} - \sigma^y_{l-1} \sigma^y_l \sigma^x_{l+1} \right) \right],$$  \hspace{1cm} (10)

where the number of the sites is $N = 2M + 1$, $\sigma^{\mu}_l (\mu = x, y, z)$ are the Pauli matrices, and the dimensionless parameter $\lambda > 0$ denotes the three-spin interaction strength (in unit of the nearest-neighbor exchange coupling). The periodic boundary condition is assumed. This model can be exactly solved by using the Jordan–Wigner transformation such as

$$\sigma^x_l = \prod_{n<l} \left( 1 - 2c_n^\dagger c_n \right) \left( c_l^\dagger + c_l \right),$$

$$\sigma^y_l = \prod_{n<l} \left( 1 - 2c_n^\dagger c_n \right) \left( c_l^\dagger - c_l \right),$$

$$\sigma^z_l = 2c_l^\dagger c_l - 1,$$  \hspace{1cm} (11)

with the operators $c_l^\dagger$, $c_l$ corresponding to the fermionic creation and annihilation operators, then along with the Fourier transformation, we can obtain the diagonalized Hamiltonian:

$$H = \sum_{k=-M}^{M} \varepsilon(\lambda, k) d_k^\dagger d_k,$$  \hspace{1cm} (12)
with the energy spectrum

\[ \varepsilon(k, \lambda) = -4 \left( \cos \theta_k - \frac{\lambda}{2} \sin 2\theta_k \right), \]  

(13)

where \( \theta_k = 2\pi k / N \). Let us give some analyses about the energy dispersion of this spinless fermion. When \( \lambda \leq 1 \), there exist two Fermi points \( \pm \theta_k^F = \pi / 2 \), which restrict the negative-energy region in the \( k \) space as \( -\theta_k^F \leq \theta_k \leq \theta_k^F \). But when the parameter \( \lambda \) exceeds the critical value \( \lambda_c = 1 \), two additional Fermi points appear at \( \theta_k^{F1} = \arcsin(1/\lambda) \), and \( \theta_k^{F2} = \pi - \arcsin(1/\lambda) \). Then there are two negative-energy regions \( -\theta_k^F \leq \theta_k \leq \theta_k^{F1} \) and \( \theta_k^{F1} \leq \theta_k \leq \theta_k^{F2} \).

In the thermodynamic limit, the GS corresponds to the configuration where all the states with \( \varepsilon(k, \lambda) \leq 0 \) are filled, and the others are empty [29]. Thus, it can be understood that when the system goes across the critical point, the structure transition of the GSs happens due to the negative-energy regions transferring. In this regard, it is naturally expected that there should occur a QPT at the critical point \( \lambda_c = 1 \). It is shown that in this system the three-spin interaction leads to a second-order QPT [29].

In the following, we start to calculate the OFS of the system. We consider the fidelity of two time evolution operators \( U(\lambda) = \exp(-it H(\lambda)) \) and \( U(\lambda + \delta \lambda) = \exp(-it H(\lambda + \delta \lambda)) \), with \( H(\lambda) \) the Hamiltonian in equation (10) and \( \delta \lambda \) denotes a tiny difference. We choose the Gibb’s thermal state \( \rho = \exp(-\beta H(\lambda))/Z(\beta, \lambda) \), where \( Z(\beta, \lambda) = \text{Tr}[\exp(-\beta H(\lambda))] \) is the partition function, and \( \beta = 1/T \) is the inverse temperature. The operators \( U \) and \( \rho \) can be written in the factorized form \( U = \bigotimes_{k=-M}^{M} U_k, \rho = \bigotimes_{k=-M}^{M} \rho_k \), where \( U_k \) is still a unitary operator and \( \rho_k \) is still a density operator, corresponding to the \( k \)th subspace. Then the operator fidelity

\[ \mathcal{F}_\rho = \left| \text{Tr}[\rho U^\dagger(\lambda + \delta \lambda)U(\lambda)] \right| \]

(14)

where \( \theta_k = 2\pi k / N \). We can also calculate the susceptibility using

\[ \chi_\rho(\lambda) = \sum_k \chi_{\rho,k}(\lambda), \]

(15)

\[ \chi_{\rho,k}(\lambda) = \text{Tr}_k[\rho_k (\partial_k U_k)^\dagger (\partial_k U_k)] - \left| \text{Tr}_k[\rho_k U_k^\dagger (\partial_k U_k)] \right|^2. \]

(16)

Thus, the susceptibility for the system with three-spin interaction is

\[ \chi_\rho(\lambda) = t^2 \sum_k \frac{\sin^2 \left( \frac{4\pi k}{N} \right)}{\cosh^2 \frac{\beta\theta_k}{2}}. \]

(17)

In the above equation, the OFS is in a square form of \( t^2 \), which is simpler than the case of the Ising model in a transverse field [21]. From the diagonalizing process, one can find that after the Jordan–Wigner and Fourier transformations, the XX chain with three-spin interaction presents
a diagonal form, i.e. consists of free fermions (see Hamiltonian (12)), while in that space the Ising chain under a transverse field is only block-diagonal (see [22]). Since we calculate the operator fidelity in the eigenspace of fermions, the diagonal form of the XX chain with three-spin interaction induces simpler results of the operator fidelity and the OFS. The sum term of equation (17) contains all the information of the system, and the temperature \( \beta = 1/T \) can be used to adjust the proportion of the eigenstates. In the following, we will study the operator fidelity and the OFS by a numerical method.

In figure 1, we numerically calculate the operator fidelity versus time \( t \). These results show the dynamical behaviors of the operator fidelity. With different interaction strength \( \lambda \), we find that when the system approaches the critical point \( \lambda_c = 1 \), the fidelity \( \mathcal{F}_\rho \) decays with time to zero and without revival. Under the larger interaction such as \( \lambda = 2 \), the fidelity \( \mathcal{F}_\rho \) oscillates with time. Weaker strength like \( \lambda = 0.6 \) will reduce \( \mathcal{F}_\rho \) much more slowly, and during longer times there will be a revival of \( \mathcal{F}_\rho \) (we do not show the very long time region). One can notice that in the shorter time region, the critical strength \( \lambda_c = 1 \) makes \( \mathcal{F}_\rho \) decay more quickly than other cases when \( \lambda \) is stronger or weaker than the critical strength \( \lambda_c \). The special behaviors of \( \mathcal{F}_\rho \) in the case \( \lambda = 1 \) reflect the critical property of the system at the point. Since we consider the low temperature case, the behavior of the operator fidelity is similar to the Loschmidt echo shown in [3].

In figure 2(a), we show the OFS versus different \( \lambda \). At a low temperature, the OFS mainly reflects the stability of the GS. Obviously, near the critical point the OFS exhibits a sharp peak. This means that when approaching the critical point \( \lambda_c = 1 \), the system is very sensitive to external perturbations. At the critical point, the system undergoes a configuration transition, which can be induced by a tiny perturbation. This is why the system is very sensitive at the critical point and the OFS can only reflect the sensitivity. One may notice the OFS in equation (17) is in terms of \( t^2 \), and we can enlarge the peak intension of OFS by properly expanding the time region. Here, we only consider the term \( \chi_\rho / t^2 \), which captures
the information of the system. The larger size \((N = 2M + 1)\) will heighten the peak value. Comparing this result to the Ising chain under transverse field \([21]\), the OFS in this model does not indicate the critical point as accurately as that in \([21]\), which also reflects the different inner configuration between the two systems. We also consider the effect of temperature on the OFS and show the results in figure 2(b). Not surprisingly, the higher temperature is not helpful to detect the QPT point, since the quantum criticality is only induced by quantum fluctuation and thermal fluctuation will cover it up. In contrast, in this system, at not very high temperature such as \(T = 0.5\), OFS can also indicate the critical point approximately. Even to the case \(T = 1\), the maximal value of OFS appears not far from the critical point. However, with increasing temperature, more effects induced by the excited states will erase the peak of OFS and give no special phenomenon at the critical point. Compared to the results in \([21, 22]\), the OFS of the Ising chain can even indicate the QPT point at the limit of \(T = \infty\). The different behaviors of the OFS reflect the different properties of the two systems under thermal fluctuation. From the results shown in figures 2(a) and (b), it is clear that the OFS can indicate the QPT point of the system effectively, and one may modulate the time and temperature to make the OFS indicate the critical point well.

4. The \((1/2, 1)\) XXZ mixed-spin chain

The above discussion can be expanded to the degenerate cases; then the density \(\rho = \sum_{n,\gamma} P_n |\Psi_{n,\gamma}\rangle \langle \Psi_{n,\gamma}|\) with the subscript \(\gamma\) denoting the degeneracy. In this section, we will consider the anisotropic \((1/2, 1)\) mixed-spin chain, which has a degenerate energy structure and abundant quantum critical behaviors \([31]\). The system under consideration consists of two kinds of spin, spin-1/2 and spin-1, alternating on a ring, with its Hamiltonian given by

\[
H = \sum_{l=1}^{N} (s'_l \cdot s'_{l+1} + S'_l \cdot s'_{l+2}) + (\Delta - 1) \sum_{l=1}^{N} (s'^z_l \cdot S'^z_{l+1} + S'^z_l \cdot s'^z_{l+2}),
\]

where \(s'_l\) and \(S'_l\) are spin-1/2 and spin-1 operators at the \(l_{th}\) site (each site contains two kinds of spins), respectively. \(N\) denotes the system size, and we only consider the even cases in this

\[\text{Figure 2.}\ (a)\ The\ \text{OFS}\ \text{divided}\ \text{by}\ t^2\ \text{versus}\ \text{different}\ \lambda\ \text{at}\ \text{the}\ \text{temperature}\ T = 0.02.\ \text{The}\ \text{different}\ \text{sizes}\ \text{of}\ \text{the}\ \text{spin}\ \text{chain}\ \text{with}\ \text{three-spin}\ \text{interaction}\ \text{are}\ \text{considered.}\ \ (b)\ \text{The}\ \text{OFS}\ \text{divided}\ \text{by}\ t^2\ \text{versus}\ \text{different}\ \lambda\ \text{with}\ \text{the}\ \text{system}\ \text{size}\ M = 1000.}\ \text{The}\ \text{cases}\ \text{of}\ \text{different}\ \text{temperatures}\ \text{are}\ \text{considered.}\\]

\[\text{the}\ \text{system}\ \text{under}\ \text{thermal}\ \text{fluctuation}\ \text{will}\ \text{cover}\ \text{it}\ \text{up}.\ \text{In}\ \text{contrast,}\ \text{in}\ \text{this}\ \text{system},\ \text{at}\ \text{not}\ \text{very}\ \text{high}\ \text{temperature}\ \text{such}\ \text{as}\ T = 0.5,\ \text{OFS}\ \text{can}\ \text{also}\ \text{indicate}\ \text{the}\ \text{critical}\ \text{point}\ \text{approximately.}\ \text{Even}\ \text{to}\ \text{the}\ \text{case}\ T = 1,}\ \text{the}\ \text{maximal}\ \text{value}\ \text{of}\ \text{OFS}\ \text{appears}\ \text{not}\ \text{far}\ \text{from}\ \text{the}\ \text{critical}\ \text{point.}\ \text{However,}\ \text{with}\ \text{increasing}\ \text{temperature,}\ \text{more}\ \text{effects}\ \text{induced}\ \text{by}\ \text{the}\ \text{excited}\ \text{states}\ \text{will}\ \text{erase}\ \text{the}\ \text{peak}\ \text{of}\ \text{OFS}\ \text{and}\ \text{give}\ \text{no}\ \text{special}\ \text{phenomenon}\ \text{at}\ \text{the}\ \text{critical}\ \text{point.}\ \text{Compared}\ \text{to}\ \text{the}\ \text{results}\ \text{in}\ [21, 22],}\ \text{the}\ \text{OFS}\ \text{of}\ \text{the}\ \text{Ising}\ \text{chain}\ \text{can}\ \text{even}\ \text{indicate}\ \text{the}\ \text{QPT}\ \text{point}\ \text{at}\ \text{the}\ \text{limit}\ \text{of}\ T = \infty.}\ \text{The}\ \text{different}\ \text{behaviors}\ \text{of}\ \text{the}\ \text{OFS}\ \text{reflect}\ \text{the}\ \text{different}\ \text{properties}\ \text{of}\ \text{the}\ \text{two}\ \text{systems}\ \text{under}\ \text{thermal}\ \text{fluctuation.}\ \text{From}\ \text{the}\ \text{results}\ \text{shown}\ \text{in}\ \text{figures}\ 2(a)\ \text{and}\ (b),}\ \text{it}\ \text{is}\ \text{clear}\ \text{that}\ \text{the}\ \text{OFS}\ \text{can}\ \text{indicate}\ \text{the}\ \text{QPT}\ \text{point}\ \text{of}\ \text{the}\ \text{system}\ \text{effectively,}\ \text{and}\ \text{one}\ \text{may}\ \text{modulate}\ \text{the}\ \text{time}\ \text{and}\ \text{temperature}\ \text{to}\ \text{make}\ \text{the}\ \text{OFS}\ \text{indicate}\ \text{the}\ \text{critical}\ \text{point}\ \text{well.}}\]

4. The \((1/2, 1)\) XXZ mixed-spin chain

The above discussion can be expanded to the degenerate cases; then the density \(\rho = \sum_{n,\gamma} P_n |\Psi_{n,\gamma}\rangle \langle \Psi_{n,\gamma}|\) with the subscript \(\gamma\) denoting the degeneracy. In this section, we will consider the anisotropic \((1/2, 1)\) mixed-spin chain, which has a degenerate energy structure and abundant quantum critical behaviors \([31]\). The system under consideration consists of two kinds of spin, spin-1/2 and spin-1, alternating on a ring, with its Hamiltonian given by

\[
H = \sum_{l=1}^{N} (s'_l \cdot s'_{l+1} + S'_l \cdot s'_{l+2}) + (\Delta - 1) \sum_{l=1}^{N} (s'^z_l \cdot S'^z_{l+1} + S'^z_l \cdot s'^z_{l+2}),
\]

where \(s'_l\) and \(S'_l\) are spin-1/2 and spin-1 operators at the \(l_{th}\) site (each site contains two kinds of spins), respectively. \(N\) denotes the system size, and we only consider the even cases in this.
study. The exchange interactions exist only between nearest neighbors, and they are of the same strength, which is set to unity. $\Delta$ is the anisotropy parameter and in this paper only the region $\Delta \geq 0$ is considered. In addition, we adopt periodic boundary conditions in the system.

In the work of Alcaraz and Malvezzi \[31\], they found that, in the region $-1 \leq \Delta < 1$, the GS of the system is single or double degenerate, and the model is in a gapless phase. However, in the Ising regime $\Delta > 1$, the GSs are of twofold degeneracy, and they have a finite energy gap in the limit of $N \to \infty$. Special properties can be expected at the isotropic point, i.e. $\Delta = 1$. At this point, the system exhibits ferrimagnetic order and the GS is highly degenerate with the degeneracy related to the system size. For example, in the $(1/2, 1)$ mixed-spin case, the GS has the degeneracy of $1 + N/2$ at the isotropic point. Therefore, the position $\Delta = 1$ is a critical point indicating the reconstruction of the energy spectrum of the system. In this work, it is expected that the operator fidelity, which is closely associated with the system structure, will present special behaviors at the critical point.

For the GSs of the system under consideration, its degeneracy is not fixed as $\Delta$ varies, so it is difficult to write an exact and convenient form of the GSs. Thus, the GS fidelity is unusable in this system. In our study, we consider the operator fidelity in a thermal mixed state, and the GS properties can be approximately represented at low enough temperature. When the temperature is low enough, the Gibb’s thermal state gives the mixture of all the degenerate GSs with equal probability, which is one of the reasonable simulation to the degenerate GS. Although this method is not an absolutely exact one, the state $\rho(T)$ can well manifest the properties of the GSs \[32\].

We consider the operator fidelity of the two time evolution operators $U(\Delta) = \exp[-itH(\Delta)]$ and $U(\Delta + \delta)$, with $H(\Delta)$ the Hamiltonian in equation \(18\) and $\delta$ denotes a tiny difference. In figure 3, we numerically study the dynamical behavior of the operator fidelity. At low temperature, one can see that the fidelity behaves as a periodic function of time; in particular, in the case of $\Delta = 1$, the fidelity oscillates more acutely than in the other cases,
\( \Delta = 0.9, 1.1 \). In the short-time region, the operator fidelity decays with time the most quickly. This phenomenon can be used to indicate the quantum critical point. In figure 4, we show the OFS versus parameter \( \Delta \) for different system sizes. With the system size up to \( N = 8 \), the peak of OFS appears close to the critical point. It tells us that at low enough temperature, the OFS of the system as large as eight spins can indicate the critical point well. Here we only consider the small size cases since, because it is generally difficult to simulate a spin chain of large length, a natural idea is to study small systems. Fortunately, small-size systems can also exhibit well properties of large-size systems such as entanglement properties [32, 33]. The numerical results in figures 3 and 4 show that the operator fidelity and its susceptibility in small systems can reflect the quantum critical properties of the anisotropy \((1/2, 1)\) mixed-spin system. When considering the thermal effect, we find that the higher temperature will cause the position of the OFS peak to move rightward. When the temperature keeps rising, the peak at the critical point will disappear. We do not show the results in this paper.

5. Conclusions

In this paper, we make use of the OFS to study the quantum critical properties. We analyze the relation between operator fidelity and GS fidelity, and find that the operator fidelity closely associates with QPT. We find that the operator fidelity corresponding to a proper state is effective to detect the first-order QPT and second-order QPT; however, the Loschmidt echo corresponding to GS cannot indicate the first-order QPT. In the isotropic spin-1/2 XX chain with three-spin interaction, we give the analytical results of operator fidelity and its susceptibility. Then we numerically study the operator fidelity, and find that when the system approaches the critical point the fidelity decays more and more quickly. At a low temperature, by modulating the strength of the three-spin interaction, the OFS presents a peak near the critical point. The nontrivial behavior of the OFS indicates the QPT. In the anisotropic \((1/2, 1)\) mixed-spin chain, by use of the thermal state we can express well the degenerate states and then we find the
operator fidelity decays sharply and oscillates acutely with time when the system tends towards the critical point. The OFS also gives a sharp peak at the critical point. The special dynamical behavior of the operator fidelity can reflect the critical properties and the OFS can indicate the critical point effectively. The operator fidelity (and OFS) is useful to characterize both the first-order QPT and the second-order QPT. It is an effective approach even in the systems with degenerate GSs. Furthermore, in experiments, one can choose proper temperature and time to make the signal of the OFS more visible. It will be interesting to make use of the operator fidelity to study KT (BKT) QPTs in other systems.

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