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Fidelity and quantum phase transitions

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Abstract
It is shown that the fidelity, a basic notion of quantum information science, may be used to characterize quantum phase transitions, regardless of what type of internal order is present in quantum many-body states. The equivalence between the existence of an order parameter and the orthogonality of different ground-state wavefunctions for a system undergoing a quantum phase transition is used to justify the introduction of the notions of irrelevant and relevant information as the counterparts of fluctuations and orders in the conventional description. The irrelevant and relevant information are quantified, which allows us to identify unstable and stable fixed points (in the sense of renormalization group theory) for quantum spin chains.

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(Some figures in this article are in colour only in the electronic version)

In recent decades, significant advances have been achieved in the study of quantum phase transitions (QPTs), both theoretically and experimentally, in systems such as high-T_c superconductors, fractional quantum Hall liquids and quantum magnets [1]. Conventionally, QPTs are characterized by singularities of the ground state energy; first-order QPTs are characterized by discontinuities in the first derivative of the energy, whereas second-order (higher-order) QPTs are characterized by discontinuities in the second (higher) derivative of the energy. At singular points, the spectrum is gapless.

The focus of the traditional description of QPTs in condensed matter physics is a Hamiltonian and its spectrum. The most studied QPTs fit into the conventional Landau–Ginzburg–Wilson (LGW) paradigm. A central concept is a local-order parameter, whose non-zero value characterizes a symmetry-breaking phase, a unique feature which only exists for a system with an infinite number of degrees of freedom, in contrast to QPTs resulting from a level crossing, which may happen in a finite-size system. However, there exist phases that are not described by symmetry-breaking orders, which results in continuous QPTs beyond the LGW paradigm [2–5]. Furthermore, a spin chain characterized by a local Hamiltonian with a matrix product ground state, where the ground state energy remains analytic, exhibits a different type of QPT from the standard paradigm [6].

On the other hand, quantum information science brings about an emerging picture which studies QPTs from the ground-state wavefunctions of systems. The cross fertilization of quantum many-body theory and quantum information science has led to fruitful outcomes. One aspect is the study of the possible role of entanglement in characterizing QPTs [7–10]. Remarkably, for quantum spin chains, the von Neumann entropy, as a bipartite entanglement measure, exhibits qualitatively different behaviors at and off criticality [9].

In this communication, we investigate the role of the fidelity, a basic notion of quantum information science, in characterizing QPTs. As a distance measure[3], the fidelity describes how close two given quantum states are. Therefore, it is natural to expect that the fidelity may be used to characterize drastic changes in quantum states when systems undergo QPTs, regardless of what type of internal order is present in quantum many-body states. The equivalence between the existence of an order parameter and the orthogonality of different ground-state wavefunctions for a system undergoing a QPT is established to justify the introduction of the notions of irrelevant and relevant information as the counterparts of fluctuations and orders in the conventional description. The irrelevant and relevant information are quantified, which allows us to identify unstable and stable fixed points (in the sense of renormalization group theory) for quantum spin chains. We present examples exhibiting a second-order phase transition, a critical line, a level crossing and an infinite-order phase transition. It is proper to stress here that Zanardi and Paunković [11] were the first to exploit the ground-state overlap, which is equivalent to the fidelity at zero temperature, to detect QPTs in the Dicke model and the XY spin chain.

We consider a quantum system S described by a Hamiltonian $H(\lambda)$, with λ a control parameter[4]. The latter may be tuned to drive the system to undergo a QPT at a transition point λ_c. At zero temperature, the system is in a ground state. The conventional characterization of QPTs is in terms of orders and fluctuations: at transition points, fluctuations are so strong that orders are destroyed, whereas away from transition points, orders survive fluctuations. Therefore (local/nonlocal) order parameters are introduced to quantify orders and fluctuations. Our first conclusion is that the presence of an order parameter is equivalent to the orthogonality between any two different ground states[5]. Indeed, if an order parameter exists for a system undergoing a QPT, then we have $\langle\psi|\phi\rangle = 0$ for any two representative ground states $|\psi\rangle$ and $|\phi\rangle$, or equivalently, the fidelity $F(\psi, \phi) \equiv |\langle\psi|\phi\rangle|$ vanishes. This is due to the fact that any representative state $|\psi\rangle$ is reliably distinguishable from another representative state $|\phi\rangle$, due to the occurrence of orders. Here the distinguishability is understood in the sense of quantum measurements; indeed, orthogonality is equivalent to state distinguishability, since two non-orthogonal states cannot be reliably distinguished, as follows from the basic postulate of quantum mechanics on quantum measurements [12]. Conversely, if the fidelity of any two ground states $|\psi\rangle$ and $|\phi\rangle$ vanishes, i.e., they are orthogonal to each other: $\langle\psi|\phi\rangle = 0$, then the equivalence between orthogonality and state distinguishability implies that there must be some physical observable, which may be exploited to distinguish the states. Therefore, this observable may be taken as an order parameter [13].

In the conventional characterization of QPTs in terms of orders and fluctuations, whether or not any two given states are in the same phase depends on whether the difference unveiled by an order parameter is quantitative or qualitative [1]. This implies that the orthogonality

[3] The fidelity is not a metric. However, the angle A between states ρ and σ defined by $A(\rho, \sigma) \equiv \arccos F(\rho, \sigma)$ is a metric [12]. That is, it is non-negative, symmetric and is equal to zero if and only if $\rho = \sigma$, and it obeys the triangle inequality: $A(\rho, \tau) \leqslant A(\rho, \sigma) + A(\sigma, \tau)$ for any states ρ, σ and τ.

[4] The extension of our discussion to systems depending on more than one parameter is straightforward.

[5] An exceptional case arises for a system with a level-crossing, in which no order emerges. However, in such a case, the states from different phases are obviously orthogonal.

between two states in the same phase results from the distinguishability due to the quantitative difference in an order parameter, which is in the short-distance details of the system, while the orthogonality between two states in different phases results from the distinguishability due to the qualitative difference in an order parameter, which reflects the long-distance behavior of the system. Since the long-distance behavior of a system does not depend on the short-distance details of the system [2], any two states in a given phase share the same long-distance behavior, with their difference characterized by the short-distance details. It is convenient to introduce the notions of relevant and irrelevant information to characterize QPTs in the context of quantum information theory. The former (latter) is the information that is encoded in the long-distance (short-distance) behavior of a given ground state. So different states in the same phase share the same relevant information, but have different irrelevant information, whereas states in different phases accommodate different relevant information.

Another description of QPTs is renormalization group (RG) theory [14], in which transition points are characterized by unstable fixed points, and ordered states are characterized by stable fixed points, with all states in a given phase flowing to a stable fixed point. Along a given RG flow, high-energy degrees of freedom are successively integrated out, whereas low-energy degrees of freedom are preserved. Therefore, irrelevant and relevant information are, respectively, the counterparts of high-energy degrees of freedom and low-energy degrees of freedom in the context of quantum information theory.

To complete our characterization of QPTs in terms of the fidelity, it is necessary to quantify irrelevant and relevant information. To this end, we restrict ourselves to considering quantum spin chains exhibiting QPTs with symmetry-breaking orders. It is known that orders in these systems emerge only in the thermodynamic limit. However, ground states are indeed boring in the sense that the fidelity for any two different ground states vanishes in the thermodynamic limit. To extract meaningful physical information, we put systems on finite chains of different sizes and study the scaling behavior of the fidelity with the system size L. In contrast to the thermodynamic limit, the fidelity for any two ground states of a finite size system does not vanish, but is exponentially decreasing with the size L.[6] That is, the fidelity $F(\lambda, \lambda')$ scales as $[d(\lambda, \lambda')]^L$, with $0 \leqslant d \leqslant 1$ a scaling parameter characterizing how fast the fidelity changes when the thermodynamic limit is approached. The scaling parameter $d(\lambda, \lambda')$ is well defined in the thermodynamic limit: $\ln d(\lambda, \lambda') = \lim_{L\to\infty} \ln F(\lambda, \lambda')/L$. *Physically, it is the average fidelity per lattice site*.

Let us discuss how the scaling parameter $d(\lambda, \lambda')$ varies with λ for a fixed λ'. Suppose the system flows to two different stable fixed points λ_- and λ_+ under RG transformations. Note that there is a loss of irrelevant information present in a state $|\psi(\lambda)\rangle$ when λ flows to a stable fixed point, although relevant information remains the same. Therefore, if λ is in the same phase as λ', we need to distinguish two cases: first, when λ approaches λ' along the flow, the loss of irrelevant information present in $|\psi(\lambda)\rangle$ makes it less distinguishable from $|\psi(\lambda')\rangle$, thus $d(\lambda, \lambda')$ monotonically increases until it reaches 1 when $\lambda = \lambda'$; second, when λ flows away from λ', the loss of irrelevant information present in $|\psi(\lambda)\rangle$ makes it more distinguishable from $|\psi(\lambda')\rangle$, thus $d(\lambda, \lambda')$ monotonically decreases along the flow. On the other hand, if λ is in a different phase from λ', then the loss of irrelevant information present in $|\psi(\lambda)\rangle$ makes it more distinguishable from $|\psi(\lambda')\rangle$, since the irrelevant information originates from the same transition point. Thus, $d(\lambda, \lambda')$ monotonically decreases with λ along the flow for a fixed λ'. Moreover, for any λ and λ', we have $d(\lambda, \lambda') \geqslant d(\lambda_-, \lambda_+)$, since two states at λ_- and λ_+ are the most distinguishable states, consistent with the fact that there is no suppression in order parameters caused from quantum fluctuations. For symmetry-breaking orders, QPTs

[6] This simply follows from the translational invariance and matrix product state representations of ground states.

Table 1. Quantum phase transitions (QPTs) from a quantum information perspective. The notions of irrelevant and relevant information are introduced to describe QPTs in terms of the fidelity, a basic notion of quantum information science, with their counterparts in the conventional theories of orders and renormalization group (RG).

Orders and fluctuations	Renormalization group flows	Fidelity
Orders	Low energy degrees of freedom	Relevant information
Fluctuations	High energy degrees of freedom	Irrelevant information
Order parameters	Effective Hamiltonians	Fidelity per lattice site
Transition points	Unstable fixed points	Pinch points
Ordered (disordered) states	Stable fixed points	Global minima

are continuous, and so is $d(\lambda, \lambda')$. But it is not analytic at $\lambda = \lambda_c$ or $\lambda' = \lambda_c$, since the relevant information in two phases is different. On the other hand, $d(\lambda, \lambda')$ is symmetric under interchange $\lambda \leftrightarrow \lambda'$, so one may recognize unstable and stable fixed points as pinch points[7] and global minima, respectively. Note that the deviation of $d(\lambda, \lambda')$ from 1 (global minima) is due to the contribution of irrelevant information if λ and λ' are from the same (different) phase(s). The connection between the fidelity approach and the conventional theories is summarized in table 1.

We remark that the above argument may be extended to other types of QPTs. However, the exponential scaling of the fidelity with the size L is not necessarily valid. Actually, for QPTs resulting from level crossings, d only takes values 0 or 1. For QPTs in matrix product systems [6], the fidelity may exhibit fast oscillating behavior with an exponentially decaying envelope. Thus *different scaling behavior signal different types of QPTs*.

Now we turn to the finite-temperature case, in which the system is in a mixed state, characterized by a density matrix ρ. A mixed state may be purified [12] if one introduces a reference system R, which has the same state space, e.g., another copy of S. That is, define a pure state $|SR\rangle$ for the joint system SR such that $\rho = \mathrm{tr}_R(|SR\rangle\langle SR|)$. Assume that orders present in ground states survive thermal fluctuations. Then we may establish the equivalence between the existence of orders and the vanishing fidelity for a system undergoing a QPT. More precisely, if an order exists, then the fidelity $F(\rho, \sigma) = \mathrm{tr}\sqrt{\rho^{1/2}\sigma\rho^{1/2}}$ vanishes for two representative states ρ and σ for a quantum system S at finite temperature. Indeed, there is an alternative characterization of the fidelity due to Uhlmann's theorem [15], which states that $F(\rho, \sigma) = \max_{|\psi\rangle, |\phi\rangle} |\langle\psi|\phi\rangle|$, where the maximization is over all purifications $|\psi\rangle$ of ρ and $|\phi\rangle$ of σ in a joint system SR, with R being a copy of S. Since *any* purifications of ρ and σ must be orthogonal to each other, due to the state distinguishability arising from the existence of an order parameter, therefore with Uhlmann's theorem, one concludes that $F(\rho, \sigma) = 0$. Conversely, if $F(\rho, \sigma) = 0$, Uhlmann's theorem implies that the purifications of ρ and σ must be orthogonal to each other, and thus they must be reliably distinguishable. Since the reference system R is fictitious, and only the system S itself is accessible, so there must be some physical observable in the system S to characterize the distinguishability of the purifications.

Quantum XY spin chain. The quantum XY spin chain is described by the Hamiltonian

$$H = -\sum_{j=-M}^{M}\left(\frac{1+\gamma}{2}\sigma_j^x\sigma_{j+1}^x + \frac{1-\gamma}{2}\sigma_j^y\sigma_{j+1}^y + \lambda\sigma_j^z\right). \qquad (1)$$

Here σ_j^x, σ_j^y and σ_j^z are the Pauli matrices at the jth lattice site. The parameter γ denotes an anisotropy in the nearest-neighbor spin–spin interaction, whereas λ is an external

[7] We define a pinch point as an intersection of two singular lines, along which four smooth pieces patch together.

magnetic field. Hamiltonian (1) may be diagonalized as $H = \sum_k \Lambda_k \left(c_k^\dagger c_k - 1\right)$, where $\Lambda_k = \sqrt{(\lambda - \cos(2\pi k/L))^2 + \gamma^2 \sin^2(2\pi k/L)}$, with c_k and $c_k^\dagger$ denoting free fermionic modes and $L = 2M + 1$. The ground state $|\psi\rangle$ is the vacuum of all fermionic modes defined by $c_k|\psi\rangle = 0$, and may be written as $|\psi\rangle = \prod_{k=1}^{M} \left(\cos(\theta_k/2) - \mathrm{i}\sin(\theta_k/2) c_k^\dagger c_{-k}^\dagger\right)|0\rangle_k |0\rangle_{-k}$, where $|0\rangle_k$ is the vacuum of the kth mode, and θ_k is defined by $\cos\theta_k = (\cos(2\pi k/L) - \lambda)/\Lambda_k$. Therefore, the fidelity F for two states $|\psi(\lambda, \gamma)\rangle$ and $|\psi(\lambda', \gamma')\rangle$ takes the form

$$F = \prod_{k=1}^{M} \cos\frac{\theta_k - \theta_k'}{2}, \tag{2}$$

where the prime denotes that the corresponding variables take their values at λ' and γ'. Obviously, $F = 1$ if $\lambda = \lambda'$ and $\gamma = \gamma'$. Generically, $\cos\frac{\theta_k - \theta_k'}{2} < 1$, therefore the fidelity decays very quickly when λ and/or γ separate, respectively, from λ' and/or γ'.

Let us first consider the Heisenberg XX model in an external magnetic field ($\gamma = 0$), with a critical line characterized by $\lambda \in [0, 1)$. In this case, $\cos\theta_k = 1$ if $\cos(2\pi k/L) \geqslant \lambda$ and $\cos\theta_k = -1$ if $\cos(2\pi k/L) < \lambda$. Therefore, if both λ and λ' are greater than 1, then we have $F = 1$, consistent with the fact that the transition point $\lambda = 1$ for the Heisenberg XX model results from a level crossing. If $\lambda > 1$ and $\lambda' \leqslant 1$ or vice versa, then $F = 0$. Suppose $\lambda < 1$ and $\lambda' < 1$, $F = 1$ only if λ and λ' are so close that there is no k satisfying $\lambda < \cos(2\pi k/L) < \lambda'$ or $\lambda' < \cos(2\pi k/L) < \lambda$. In the thermodynamic limit, such a k always exists irrespective of λ and λ'. That is, $F = 0$ except for $\lambda = \lambda'$, indicating that there is a line of critical points $[0, 1)$, identified as the Luttinger liquids with the dynamical critical exponent $z = 1$. We stress that the transition point $\lambda_c = 1$ with $z = 2$ controls the global features of the system.

Next consider the quantum transverse Ising universality class with the critical line $\gamma \neq 0$ and $\lambda = 1$. There is only one (second-order) critical point $\lambda_c = 1$ separating two gapful phases: (spin reversal) Z_2 symmetry-breaking and symmetric phases. In the thermodynamic limit, the scaling parameter d takes the form: $\ln d(\lambda, \lambda') = 1/(2\pi) \int_0^\pi \mathrm{d}\alpha \ln \mathcal{F}(\lambda, \lambda'; \alpha)$, where $\mathcal{F}(\lambda, \lambda'; \alpha) = \cos[\vartheta(\lambda; \alpha) - \vartheta(\lambda'; \alpha)]/2$, with $\cos\vartheta(\lambda; \alpha) = (\cos\alpha - \lambda)/\sqrt{(\cos\alpha - \lambda)^2 + \gamma^2 \sin^2\alpha}$. We plot d in figure 1 for the transverse Ising model ($\gamma = 1$). One observes that the transition point $\lambda_c = 1$ is characterized as a pinch point $(1, 1)$ and that the two stable fixed points at $\lambda = 0$ and $\lambda = \infty$ are characterized as the global minima, which take value $1/\sqrt{2}$ at $(0, \infty)$ and $(\infty, 0)$.

The last case is the disorder line, i.e., a unit circle given by $\lambda^2 + \gamma^2 = 1$ in the λ–γ plane. We plot the scaling parameter d in figure 2, from which one may read off that there are two transition points $(\pm 1, 0)$ and that there are two phases corresponding to the upper and lower semi-circles, with $(0, \pm 1)$ as stable fixed points. The latter corresponds to two states with all spins aligning in the x and y directions, respectively. The system is dual to a spin-1/2 model with three-body interactions

$$H = \sum_i 2(g^2 - 1)\sigma_i^z \sigma_{i+1}^z - (1 + g)^2 \sigma_i^x + (g - 1)^2 \sigma_i^z \sigma_{i+1}^x \sigma_{i+2}^z, \tag{3}$$

with $\lambda = (1 - g^2)/(1 + g^2)$, $\gamma = 2g/(1 + g^2)$. As shown in ref. [6], the model exhibits a peculiar QPT in the thermodynamic limit, with divergent correlation length, vanishing energy gap, but analytic ground-state energy. We emphasize that the parameter space should be compactified by identifying $g = +\infty$ and $g = -\infty$, due to the fact that $H(+\infty) = H(-\infty)$. Since ground states are matrix product states [6], it is straightforward to get the fidelity F for two states $|\psi(g)\rangle$ and $|\psi(g')\rangle$,

$$F = \frac{|(1 + \sqrt{gg'})^L + (1 - \sqrt{gg'})^L|}{\sqrt{[(1 + g)^L + (1 - g)^L][(1 + g')^L + (1 - g')^L]}}. \tag{4}$$

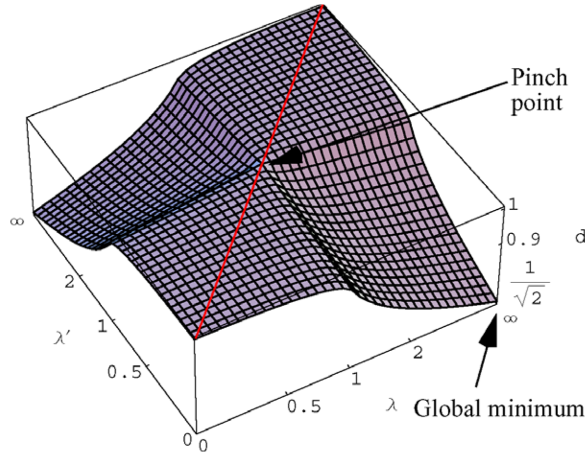

Figure 1. The scaling parameter d, which appears in the fidelity scaling $F(\lambda, \lambda') \sim d^L$, for the two states of quantum transverse Ising model as a function of λ and λ'. The transition point $\lambda_c = 1$ is characterized as a pinch point (1, 1) and the two stable fixed points, to which all states in two phases flow, are characterized as the global minima at $(0, \infty)$ and $(\infty, 0)$. The red line denotes $d(\lambda, \lambda) = 1$.

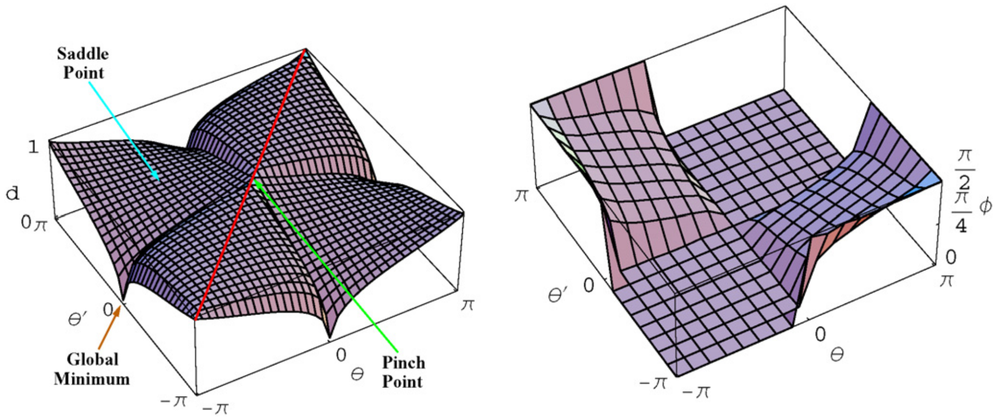

Figure 2. For the disorder line, $\lambda^2+\gamma^2 = 1$ parameterized as $\lambda = \cos\theta$, and $\gamma = \sin\theta$, the fidelity $F(\theta, \theta')$ scales as $d^L cos(L\phi)$. Thus for $\phi \neq 0$, there is a sinusoidal oscillation with an exponential envelope in the fidelity. Left: the scaling parameter d as a function of θ and θ', displaying pinch points at $(\theta, \theta') = (0, 0)$ and (π, π), and saddle points at $(\pi/2, -\pi/2)$ and $(-\pi/2, \pi/2)$, if one identifies π with $-\pi$. The pinch points characterize the two transition points, while the saddle points characterize the stable fixed points, to which all states in two phases flow. The global minima at $(0, \pi)$ and $(\pi, 0)$ correspond to the transition points, due to the fact that both irrelevant and relevant information are different. Right: the phase ϕ as a function of θ and θ'.

The fidelity F decays exponentially for two states in the same phase, but it is oscillating very fast with exponentially decaying envelope for two states in different phases. From this one may extract the scaling parameter d as $d(g, g') = \sqrt{1 + |gg'|}/\sqrt{(1 + |g|)(1 + |g'|)}$ if g and g' are in different phases, and $d(g, g') = (1 + \sqrt{|gg'|})/\sqrt{(1 + |g|)(1 + |g'|)}$ if g and g' are in the same phase. There are two transition points, i.e., $g = 0$ and ∞. All states for positive g flow to the product state ($g = 1$) with all spins aligning in the x direction, and all states for negative g flow to the cluster state [16] ($g = -1$).

In summary, we have established an intriguing connection between the fidelity and QPTs in particular and between quantum information science and condensed matter physics in general.

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References

[1] Sachdev S 1999 *Quantum Phase Transitions* (Cambridge: Cambridge University Press)
[2] Wen X-G 2004 *Quantum Field Theory of Many-Body Systems* (Oxford: Oxford University Press)
[3] Wen X-G and Wu Y-S 1993 *Phys. Rev. Lett.* **70** 1501
Senthil T, Marston J B and Fisher M P A 1999 *Phys. Rev.* B **60** 4245
[4] Senthil T *et al* 2004 *Science* **303** 1490
[5] Ran Y and Wen X-G 2006 *Phys. Rev. Lett.* **96** 026802
[6] Wolf M *et al* 2006 *Phys. Rev. Lett.* **97** 110403
[7] Preskill J 2000 *J. Mod. Opt.* **47** 127
[8] Osborne T J and Nielsen M A 2002 *Phys. Rev.* A **66** 032110
Osterloh A *et al* 2002 *Nature* **416** 608
[9] Vidal G *et al* 2003 *Phys. Rev. Lett.* **90** 227902
[10] Kitaev A and Preskill J 2005 arXiv:hep-th/0510092
Levin M and Wen X-G 2005 arXiv:cond-mat/0510613
[11] Zanardi P and Paunković N 2006 *Phys. Rev.* E **74** 031123
[12] Nielsen M A and Chuang I L 2000 *Quantum Computation and Quantum Information* (Cambrige: Cambridge University Press)
[13] A systematic way to extract order parameters directly from ground-state wave functions was proposed recently in Furukawa S, Misguich G and Oshikawa M 2006 *Phys. Rev. Lett.* **96** 047211
[14] Cardy J 1996 *Scaling and Renormalization in Statistical Mechanics* (Cambridge: Cambridge University Press)
[15] Uhlmann A 1976 *Rep. Math. Phys.* **9** 273
[16] Raussendorf R and Briegel H J 2001 *Phys. Rev. Lett.* **86** 910