This is the accepted manuscript made available via CHORUS. The article has been published as:

Quantum Fidelity in the Thermodynamic Limit

Marek M. Rams and Bogdan Damski

Phys. Rev. Lett. **106**, 055701 — Published 4 February 2011

DOI: 10.1103/PhysRevLett.106.055701

Quantum fidelity in the thermodynamic limit

Marek M. Rams[1,2] and Bogdan Damski[1]
[1] *Los Alamos National Laboratory, Theoretical Division, MS B213, Los Alamos, NM, 87545, USA*
[2] *Institute of Physics, Jagiellonian University, Reymonta 4, PL-30059 Kraków, Poland*

We study quantum fidelity, the overlap between two ground states of a many-body system, focusing on the thermodynamic regime. We show how drop of fidelity near a critical point encodes universal information about a quantum phase transition. Our general scaling results are illustrated in the quantum Ising chain for which a remarkably simple expression for fidelity is found.

PACS numbers: 64.70.Tg,03.67.-a,75.10.Jm

REVIEW COPY
NOT FOR DISTRIBUTION

A quantum phase transition (QPT) happens when dramatic changes in the ground state properties of a quantum system can be induced by a tiny variation of an external parameter [1]. This external parameter can be a strength of a magnetic field in spin systems (e.g. Ising chains [2] and spin-1 Bose-Einstein condensates [3]), intensity of a laser beam creating a lattice for cold atom emulators of Hubbard models [4], or dopant concentration in high-Tc superconductors [5]. At the heart of the sharp transition lies non-analyticity of the ground state wave-function across the critical point separating the two phases. QPTs, traditionally associated with condensed matter physics, are nowadays intensively studied from the quantum information perspective (see e.g. [6]).

Quantum fidelity – also referred to as fidelity – is a popular concept of quantum information science defined here as the overlap between two quantum states

$$\mathcal{F}(g,\delta) = |\langle g-\delta|g+\delta\rangle|, \tag{1}$$

where $|g\rangle$ is a ground state wave-function of a many-body Hamiltonian $\hat{H}(g)$ describing the system exposed to an external field g, and δ is a small parameter difference. It provides the most basic probe into the dramatic change of the wave-function near and at the critical point [7].

The recent surge in studies of fidelity follows discovery that quantum criticality promotes decay of fidelity [7]. This is in agreement with the intuitive picture of a QPT: as system properties change dramatically in the neighborhood of the critical point, ground state wave-function taken at different values of the external parameter – $|g-\delta\rangle$ and $|g+\delta\rangle$ – have little in common and so their overlap decreases.

As fidelity is given by the angle between two vectors in the Hilbert space, it is a geometric quantity [8]. Thus, it has been proposed as a robust geometric probe of quantum criticality applicable to all systems undergoing a QPT *regardless* of their symmetries and order parameters whose prior knowledge is required in traditional approaches to QPTs. Fidelity has been recently studied in this context in several models of condensed matter physics (see [9] and references therein).

Besides being an efficient probe of quantum criticality, fidelity appears in numerous problems in quantum physics. Indeed, it is related to density of topological defects after a quench [10–12], decoherence rate of a test qubit interacting with an out-of-equilibrium environment [13], orthogonality catastrophe of condensed matter systems (see [14] and the references citing it). Therefore its understanding has an interdisciplinary impact.

To unravel the influence of quantum criticality on fidelity, one has to determine if its drop near the critical point encodes universal information about the transition in addition to providing the location of the critical point. This universal information is given by the critical exponents and reflects symmetries of the model rather than its microscopic details. In the "small system limit", which broadly speaking corresponds to $\delta \to 0$ at fixed system size N, the answer is positive. This is explored in the fidelity susceptibility approach where [7, 9, 15]

$$\mathcal{F}(g,\delta) \simeq 1 - \delta^2\chi_F(g)/2, \tag{2}$$

and χ_F stands for fidelity susceptibility. Universal information, or simply the critical exponent ν, is encoded in its scaling: at the critical point $\chi_F(g_c) \sim N^{2/d\nu}$, while far away from it $\chi_F(g) \sim N|g-g_c|^{d\nu-2}$, where d is system dimensionality [11, 12, 16].

In the thermodynamic limit, which broadly speaking corresponds to $N \to \infty$ at fixed δ, the answer is positive as well. This is our key result stating that

$$\ln \mathcal{F}(g,\delta) \simeq -N|\delta|^{d\nu} A\left(\frac{g-g_c}{|\delta|}\right), \tag{3}$$

where A is a scaling function. In particular, we see that fidelity is non-analytic in δ at the critical point, $\ln \mathcal{F}(g_c,\delta) \sim -N|\delta|^{d\nu}$, while away from it, i.e., for $|\delta| \ll |g-g_c| \ll 1$, we obtain

$$\ln \mathcal{F}(g,\delta) \sim -N\delta^2|g-g_c|^{d\nu-2}, \tag{4}$$

after expansion of the scaling function. These results, in particular, set firm foundations for usage of fidelity as a probe of quantum criticality in thermodynamically-large systems. In the context of theoretical studies of QPTs, the strength of the fidelity approach lies in its simplicity: all information encoded in the ground state wave-function(s) is "compactified" into a single number.

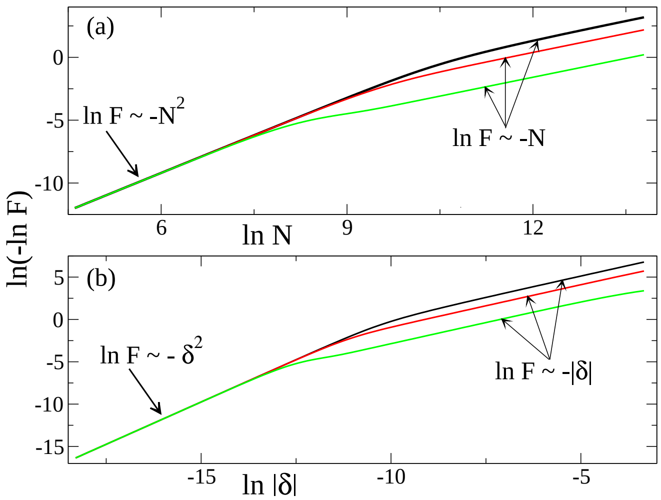

FIG. 1: (color online) Fidelity of the Ising chain near the critical point as a function of (a) the system size N at fixed $\delta = 10^{-4}$ and (b) parameter difference δ at the fixed system size $N = 10^5$. On both panels the curves from top to bottom correspond to $\mathcal{F}(1,\delta)$, $\mathcal{F}(1+\delta,\delta)$ and $\mathcal{F}(1+5\delta,\delta)$.

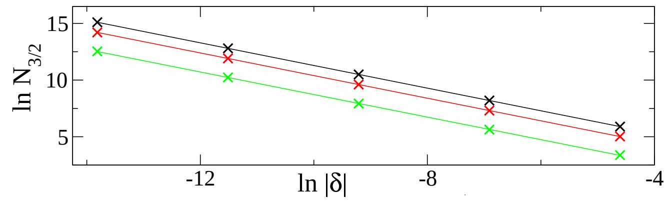

FIG. 2: (color online) Study of the crossover between the "small system limit" and the thermodynamic limit illustrated in Fig. 1. As the system size is increased in Fig. 1a, the slope of the curves changes smoothly from 2 (corresponding to $\ln\mathcal{F} \sim -N^2$) to 1 (corresponding to $\ln\mathcal{F} \sim -N$). The crossover region between the two limits is centered around $N = N_{3/2}$ where the slope equals 3/2. To find it, we have calculated numerically $\mathcal{F}(g,\delta)$ vs. N – as in Fig. 1a – for various δ's and found that $N_{3/2}|\delta| \sim 1$. This is illustrated in this figure where data sets from top to bottom correspond to results obtained for $g = 1$, $1+\delta$ and $1+5\delta$, respectively (similarly as in Fig. 1a). The power-law fits (straight lines) to numerical data (crosses) give $N_{3/2} = a|\delta|^{-b}$, where $b = 0.995 \pm 0.003$ for all three fits, while the prefactor a changes between the fits from 3.6 to 0.3. Similar analysis can be done on curves shown in Fig. 1b providing the same result. Thus we conclude that the crossover condition reads $N|\delta| \sim 1$ near the Ising critical point.

A competing approach for extraction of the exponent ν – study of the asymptotic decay of correlation functions to obtain the correlation length – is considerably more complicated. Below we illustrate these predictions on the paradigmatic model of quantum phase transitions, the Ising chain, and discuss the scaling theory that leads to (3) and (4).

The Hamiltonian of the one dimensional Ising chain reads [1]

$$\hat{H}(g) = -\sum_{i=1}^{N}(\sigma_i^x\sigma_{i+1}^x + g\sigma_i^z),$$

where g stands for a magnetic field acting along the z direction. Above the spin-spin interactions try to enforce $\pm x$ polarization of spins, while the magnetic field tries to polarize spins along its direction ($+z$ for $g > 0$). This competition results in two critical points at $g_c = \pm 1$: the system is in the ferromagnetic (paramagnetic) phase for $-1 < g < 1$ ($|g| > 1$). The critical exponent $\nu = 1$. This model is solved by mapping spins onto non-interacting fermions via the Jordan-Wigner transformation [1].

Behavior of fidelity (1) around the critical point, $g \approx g_c$, is summarized in Fig. 1. In Fig. 1a the parameter difference δ is kept fixed and the system size is increased. For small system sizes we reproduce the known result, $\ln\mathcal{F} \sim -N^2$ [7], resulting from finite size scaling effects (see e.g. [9, 11, 12, 16]). For large system sizes, however, we obtain $\ln\mathcal{F} \sim -N$ in agreement with (3) and the fidelity per site approach [17–19]. As is shown in Fig. 2, the transition between the two regimes takes place when

$$N|\delta| \sim 1, \quad (5)$$

which will be discussed below.

Similarly, we observe two distinct regimes when the system size N is kept fixed and the parameter difference δ is varied (Fig. 1b). For $N|\delta| \ll 1$ we observe $\ln\mathcal{F} \sim -\delta^2$, in agreement with (2), while for $N|\delta| \gg 1$ we find $\ln\mathcal{F} \sim -|\delta|$ in agreement with (3). In the latter fidelity *approaches* non-analytic limit (where $\partial_\delta\mathcal{F}$ at $\delta = 0$ is undefined) reflecting singularities of the ground state wave-function resulting from the QPT [20].

We also see on both panels of Fig. 1 that all curves collapse for $N|\delta| \ll 1$, while they stay distinct in the opposite limit. Thus, for $N|\delta| \gg 1$ sensitivity of fidelity to quantum criticality is enhanced. This can be understood if we focus on Fig. 1a: in the large N limit dramatic changes in the ground state wave-function near the critical point are expected.

As analytical results for fidelity are scarce, we find it remarkable that we can derive accurate analytical description in the complicated limit of $N|\delta| \gg 1$, where the Taylor expansion (2) fails. To proceed, we calculate $\mathcal{F}(1+\epsilon,\delta)$, where ϵ measures distance from the critical point. For the Ising chain $\mathcal{F} = \Pi_{k>0} f_k$, where $f_k = \cos(\theta_+(k)/2 - \theta_-(k)/2)$ and $\tan(\theta_\pm(k)) = \sin k/(1+\epsilon \pm \delta - \cos k)$. We stay close to the critical point so that $0 \le |\delta|, |\epsilon| \ll 1$ and introduce natural parameterization: $c = \epsilon/|\delta|$. Taking the limit of $N \to \infty$ at *fixed* δ the product $\Pi_k f_k$ can be changed into $\exp(N\int dk \ln f_k/2\pi)$, which can be further simplified to

$$\ln\mathcal{F} \simeq -N|\delta|A(c) \quad (6)$$

in the leading order in δ and ϵ. This result is in prefect

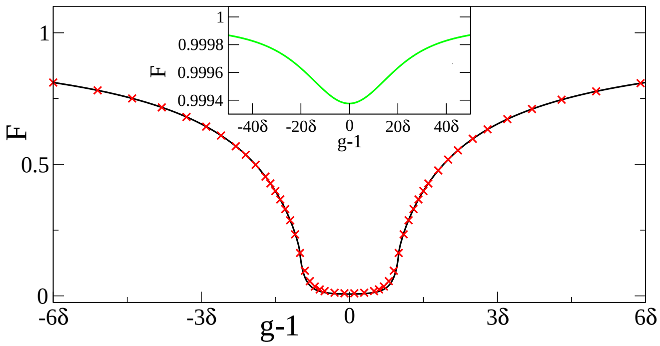

FIG. 3: (color online) Fidelity $\mathcal{F}(g,\delta)$ of the Ising chain near the critical point: thermodynamic limit (main plot) vs. "small system limit" (inset). Main plot: black curve is our analytic approximation (6), while red crosses come from numerics. Both were obtained for $N = 2\times10^5$ and $\delta = 10^{-4}$ ($N|\delta| \gg 1$). Inset: numerical result for $N = 10^3$ and $\delta = 10^{-4}$ ($N|\delta| \ll 1$). In the "small system limit" fidelity stays close to unity at any distance from the critical point, while in the thermodynamic limit it can interpolate between zero and unity.

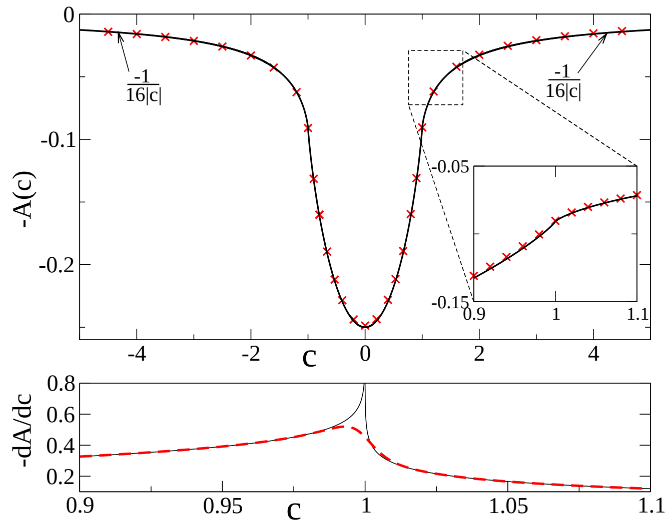

FIG. 4: (color online) Upper plot: scaling function $A(c)$ of the Ising chain. The solid black line provides the analytic result (7), while the red crosses show numerics (i.e., $\ln\mathcal{F}/N|\delta|$). The inset highlights singularity at $c = 1$. Lower plot: logarithmic divergence of $dA/dc|_{c=1}$ discussed in the text. The solid black line is the derivative of (7), while the red dashed line is a numerical result: the difference between the two near the pinch point at $c = 1$ is due to the finite system size N [19]. It disappears in the limit of $N \to \infty$. In both plots numerics is done for $N = 10^5$ and $\delta = \pi 10^{-3}$.

agreement with our universal scaling law (3): note that $\nu, d = 1$ in our model and $c = (g - g_c)/|\delta|$. Moreover, it agrees well with exact numerical simulations: Fig. 3. Above $A(c)$ is given by

$$A(c) = \begin{cases} \dfrac{1}{4} + \dfrac{|c|K(c_1)}{2\pi} + \dfrac{(|c|-1)\mathrm{Im}E(c_2)}{4\pi}; |c| \le 1 \\ \dfrac{|c|}{4} - \dfrac{|c|K(c_1)}{2\pi} - \dfrac{(|c|-1)\mathrm{Im}E(c_2)}{4\pi}; |c| > 1. \end{cases} \tag{7}$$

where $c_1 = -4|c|/(|c|-1)^2$, $c_2 = (|c|+1)^2/(|c|-1)^2$, and K and E are complete elliptic integrals of the first and second kind, respectively. Agreement between (7) and numerics is very good: see Fig. 4 for detailed comparison of $A(c)$ to numerics. Several interesting results can be obtained now.

First, Eq. (6) shows analytically how the so-called Anderson catastrophe – disappearance of the overlap between distinct ground states of an infinitely large many-body quantum system [14] – happens in the Ising chain.

Second, Eq. (6) explains the lack of collapse of the various curves providing fidelity around the critical point in the $N|\delta| \gg 1$ limit. Indeed, fidelity calculated for two ground states symmetrically around the critical point is $\mathcal{F}(1,\delta) \simeq \exp(-N|\delta|/4)$, but if one of the ground states is obtained at the critical point, $\mathcal{F}(1\pm\delta,\delta) \simeq \exp(-N|\delta|(\pi-2)/4\pi)$. In the opposite limit of $N|\delta| \ll 1$, $\mathcal{F} \simeq 1 - \delta^2 N^2/16$ in both cases explaining the collapse of all curves in this limit in Fig. 1.

Third, there is a singularity in the derivative of fidelity when one of the states is calculated at the critical point: $d\mathcal{F}(g\pm\delta,\delta)/dg|_{g=g_c=1}$ is divergent when $N \to \infty$ at fixed δ. This reflects singularity of the wave-function at the critical point approached in the thermodynamic limit. Quantitatively, $dA(c)/dc|_{c\to1^\pm} = \ln|1-c|/4\pi - 3\ln 2/4\pi + (1\pm1)/8 + \mathcal{O}((1-c)\ln|1-c|)$, which is logarithmically divergent at $c = 1$ (Fig. 4). This divergence is a signature of a pinch point found in [17–19] when fidelity between two distinct ground states states was studied. The logarithmic divergence in the Ising chain was numerically observed in [19].

Last but not least, we obtain from (6) a compact expression for fidelity away from the critical point. Taking $|c| \gg 1$ (but still $|\epsilon| = |c\delta| \ll 1$), $A(c) \simeq 1/16|c|$ and so

$$\mathcal{F} \;\simeq\; \exp(-N\delta^2/16|\epsilon|), \tag{8}$$

in agreement with (4). This reduces to a known result for fidelity susceptibility when the argument of the exponent is small and so $\mathcal{F} \simeq 1 - \delta^2 N/16|\epsilon|$ (see e.g. [9]), but provides a new result in the opposite limit where lowest order of the Taylor expansion is insufficient. We notice also that (8) is analytical in δ even in the limit of $N \to \infty$: there are no singularities expected when the system is far away from the critical point.

Below we derive general scaling results (3) and (4). This can be done by studying the scaling parameter

$$\tilde{d}(g+\delta, g-\delta) = -\lim_{N\to\infty} \ln\mathcal{F}(g,\delta)/N,$$

introduced in [17] in the context of fidelity per site approach to the thermodynamic limit. We expect that this limit is reached when

$$\min[(\xi(g+\delta), \xi(g-\delta)] \ll L, \tag{9}$$

where $\xi(g)$ is the correlation length at magnetic field g and L is the linear size of the system ($N = L^d$ for a d-dimensional system). Indeed, the smaller of the two correlation lengths sets the scale on which the states entering fidelity "monitor" each other (1). In particular, it explains our results showing that the thermodynamic limit is reached even when one of the states is calculated at the critical point and so its correlation length is infinite. Near a critical point (9) is equivalent to $L|\delta|^\nu \gg 1$ [21]. For the Ising chain studied above it reads $N|\delta| \gg 1$ properly predicting the crossover condition (5) obtained from numerical simulations (Fig. 2).

Generalizing the scaling theory of second order QPTs (Sec. 1.4 of [22]), we propose the following scaling ansatz for the universal part of the scaling parameter

$$\tilde{d}(g_c + \epsilon + \delta, g_c + \epsilon - \delta) = b^{-d} f((\epsilon + \delta)b^{1/\nu}, (\epsilon - \delta)b^{1/\nu}),$$

where f is the scaling function, b is the scaling factor, and ν is the critical exponent providing divergence of the coherence length $\xi \sim |g - g_c|^{-\nu}$. The scaling function depends on both $\epsilon + \delta$ and $\epsilon - \delta$ as they are renormalized simultaneously. The factor b^{-d} appears for dimensional reasons. Scaling of $\epsilon + \delta$ and $\epsilon - \delta$ is given by scaling of the correlation length $\xi(\epsilon \pm \delta) = b\xi((\epsilon \pm \delta)b^{1/\nu})$.

Taking $g = g_c + \epsilon$, introducing natural parameterization $\epsilon = c|\delta|$, and fixing the scale of renormalization through $|\delta|b^{1/\nu} = 1$ we obtain $\tilde{d}(g + \delta, g - \delta) = |\delta|^{d\nu} f(c + 1, c - 1)$. It gives (3) after setting $f(c + 1, c - 1) = A(c)$. In a general context, (3) shows how universal part of the scaling parameter causes the Anderson catastrophe near a critical point.

The scaling function $A(c)$ can be simplified away from the critical point. We assume below $\epsilon, \delta > 0$ for simplicity, take $\delta \ll \epsilon \ll 1$, and set b through $(\epsilon + \delta)b^{1/\nu} = 1$ exploring the freedom to choose the renormalization scale. Simple calculation results in $\tilde{d}(g + \delta, g - \delta) = (\epsilon + \delta)^{d\nu} f(1, (\epsilon - \delta)/(\epsilon + \delta))$, where the second argument of f is close to unity. Expanding f in it we get $\tilde{d}(g + \delta, g - \delta) \approx 2\delta^2 \epsilon^{d\nu - 2} f''(1, x)|_{x=1}$ as $f(1, x)$ has a minimum equal to zero at $x = 1$. Thus, away from a critical point we end up with (4). When the system is small enough, $N\delta^2|\epsilon|^{d\nu-2} \ll 1$, but still in the thermodynamic limit (9), we reproduce the known result for fidelity susceptibility $1 - \mathcal{F} \sim \delta^2 N|\epsilon|^{d\nu-2}$ [11, 12, 16]. Otherwise, (4) provides a new result.

On general grounds, one can expect that for systems with $d\nu \geq 2$ non-universal (system-specific) corrections to the above scaling relations may be significant [12], which requires further investigation.

Summarizing, our work characterizes fidelity – a modern probe of quantum criticality – in the thermodynamic limit. We have derived, and verified on a specific model, new universal scaling properties of fidelity. These findings should be experimentally relevant as the first experimental studies of ground state fidelity have been already done [23].

This work is supported by U.S. Department of Energy through the LANL/LDRD Program.

[1] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, U.K., 1999).
[2] R. Coldea *et al.*, Science **327**, 177 (2010).
[3] L.E. Sadler *et al.*, Nature (London) **443**, 312 (2006).
[4] M. Greiner *et al.*, Nature (London) **415**, 39 (2002); R. Jördens *et al.*, Nature (London) **455**, 204 (2008); M. Lewenstein *et al.*, Adv. Phys. **56**, 243 (2007).
[5] P. A. Lee, N. Nagaosa, and X.-G. Wen, Rev. Mod. Phys. **78**, 17 (2006).
[6] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).
[7] P. Zanardi and N. Paunković, Phys. Rev. E **74**, 031123 (2006).
[8] P. Zanardi, P. Giorda, and M. Cozzini, Phys. Rev. Lett. **99**, 100603 (2007).
[9] S.-J. Gu, ArXiv e-prints (2008), 0811.3127.
[10] B. Damski, Phys. Rev. Lett. **95**, 035701 (2005).
[11] R. A. Barankov, ArXiv e-prints (2009), 0910.0255.
[12] V. Gritsev and A. Polkovnikov, in *Understanding in Quantum Phase Transitions* edited by L. Carr (Taylor & Francis, Boca Raton, 2010); arXiv:0910.3692.
[13] B. Damski, H. T. Quan, and W. H. Zurek, ArXiv e-prints (2009), 0911.5729.
[14] P. W. Anderson, Phys. Rev. Lett. **18**, 1049 (1967).
[15] W.-L. You, Y.-W. Li, and S.-J. Gu, Phys. Rev. E **76**, 022101 (2007).
[16] A. F. Albuquerque, F. Alet, C. Sire, and S. Capponi, Phys. Rev. B **81**, 064418 (2010).
[17] H. Zhou and J. P. Barjaktarevič, J. Phys. A **41**, 412001 (2008).
[18] H. Zhou, R. Orús, and G. Vidal, Phys. Rev. Lett. **100**, 080601 (2008).
[19] H. Zhou, J. Zhao, and B. Li, J. Phys. A **41**, 492002 (2008).
[20] In a finite system we expect fidelity to be analytic as there are no singularities in the ground state wave-functions of finite systems. As we discuss in the Letter, there are conditions under which the leading order contribution to fidelity is non-analytic and finite size corrections rounding off singularities are barely visible (Fig. 1b). If the system is in this regime, it *approaches* the non-analytic limit.
[21] The opposite limit, $L|\delta|^{\nu} \ll 1$, provides a condition for validity of the fidelity susceptibility approach near the critical point (see e.g. [11, 12]).
[22] M. A. Continentino, *Quantum Scaling in Many-Body Systems* (World Scientific Publishing, Singapore, 2001).
[23] J. Zhang *et al.*, Phys. Rev. Lett. **100**, 100501 (2008); J. Zhang *et al.*, Phys. Rev. A **79**, 012305 (2009).