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 present novel analytical results for quantum fidelity of the Ising chain – a paradigmatic model of quantum phase transitions – and discuss a theory extending these findings to systems characterized by other universality classes. In particular, we show how quantum fidelity approaches a non-analytic limit and discuss scaling properties of quantum fidelity when it cannot be approximated by the popular fidelity susceptibility approach.

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

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). Moreover, it has been recently linked to the interdisciplinary field of dynamics of QPTs [10] in studies of both the sudden quench [11, 12] and critical dynamics of decoherence [13].

Exact analytical results for fidelity are typically unavailable, with an exception provided by ground states expressible through some matrix product states [14]. Thus, advanced numerical techniques have been employed including tensor networks [15] and quantum Monte Carlo simulations [16].

A standard approximation uses Taylor expansion of the ground state wave function in $\delta \to 0$: $|g+\delta\rangle = \sum_n \delta^n \partial_g^n |g\rangle/n!$ leading in the lowest order to [7, 9, 17]

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

where χ_F defines fidelity susceptibility. Fidelity susceptibility, unlike fidelity, is a local quantity independent of the parameter shift δ. It is thus easier to analyze than fidelity. Similarly as fidelity, χ_F is sensitive to criticality. Thus, it was proposed and studied as a probe of quantum critical properties [7, 9, 17].

Other approach focuses on studies of fidelity per site [15, 18, 19]. It was proposed in this context that one can investigate the overlap between any two ground states and the quantum criticality will be revealed by the pinch points appearing when fidelity is calculated between a critical and a non-critical ground state. The pinch point is characterized by divergence of the derivative of fidelity.

We show that when the popular expansion (2) breaks, the system enters a regime where new universal scaling properties of fidelity emerge. For example, fidelity approaches a non-analytic function of δ there [20]. This can be intuitively understood when we fix g and δ, such that both states entering (1) are obtained near the critical point, and vary the system size N. As singularities in the wave-function arise for $N \to \infty$, we expect (2) to work well for small systems. For large ones, however, the wave-function approaches the non-analytic limit and fidelity shall reflect it [20]. Thus, on general grounds, we predict that there is a fundamental change in the functional dependence of fidelity around the critical point when the system size increases. We illustrate this prediction on a

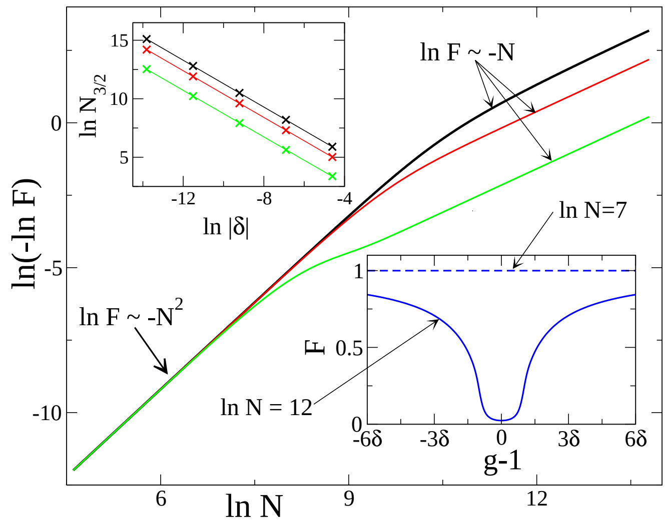

FIG. 1: (color online) Fidelity of the Ising chain near the critical point as a function of the system size N at fixed $\delta = 10^{-4}$. The curves from top to bottom correspond to $\mathcal{F}(1,\delta)$, $\mathcal{F}(1+\delta,\delta)$ and $\mathcal{F}(1+5\delta,\delta)$ (1). As the system size is increased, the slope of the curves changes smoothly from 2 to 1. The crossover region between the two limits is at $N = N_{3/2}$ where the slope equals 3/2. To numerically locate it, we have calculated $\mathcal{F}(1,\delta)$, $\mathcal{F}(1+\delta,\delta)$ and $\mathcal{F}(1+5\delta,\delta)$ – as in the main figure – for various δ's and found that the crossover condition is reached for $N_{3/2}|\delta| \sim 1$. This is illustrated in the upper inset where the power-law fits (straight lines) to numerical data (crosses) give $N_{3/2} = (0.3 \div 3.6)/|\delta|^{0.995\pm0.003}$. Order of the curves in the upper inset is the same as on the main plot. Lower inset shows that fidelity stays close to unity for small systems (dashed line calculated for $\ln N = 7$) and explores all the values between zero and unity when system size increases (solid line calculated for $\ln N = 12$). Our theory, Eq. (4), *perfectly* overlaps with the latter numerical result on the scales explored in the lower inset.

specific example, the quantum Ising model, and develop a scaling theory to generalize the Ising model-findings to other critical systems.

The Hamiltonian of the 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 exponents are $z, \nu = 1$. This model is solved in a standard way 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 Figs. 1 and 2. In the first figure 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 qualitative agreement with the fidelity per site approach [15, 18, 19]. As shown in Fig. 1, the transition between the two regimes takes place when

$$N|\delta| \sim 1 \tag{3}$$

(a theory explaining this result will be outlined below).

Similarly, we observe two distinct regimes when the system size N is kept fixed and the parameter difference δ is varied (Fig. 2). 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 the latter fidelity *approaches* non-analytic limit (where $\partial_\delta\mathcal{F}$ at $\delta = 0$ is undefined) reflecting singularities associated with the QPT [20].

We also see on both figures 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. 1: 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

$$\ln\mathcal{F} \;\simeq\; -N|\delta|A(c) \tag{4}$$

in the leading order in δ and ϵ. Above $A(c)$ is given by

$$A(c) = \begin{cases} \dfrac{1}{4} + \dfrac{|c|K(c_1)}{2\pi} + \dfrac{(|c|-1)\mathrm{Im}E(c_2)}{4\pi}; |c| \le 1 \\ \dfrac{|c|}{4} - \dfrac{|c|K(c_1)}{2\pi} - \dfrac{(|c|-1)\mathrm{Im}E(c_2)}{4\pi}; |c| > 1. \end{cases} \tag{5}$$

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 (4) and numerics is very good: see Fig. 3 for detailed comparison of $A(c)$ to numerics as well as Figs. 1 and 2. Several interesting results can be obtained from (4).

First, Eq. (4) shows analytically how the so-called Anderson catastrophe – disappearance of the overlap between distinct ground states of an infinitely large many-body quantum system [21] – happens in the Ising chain.

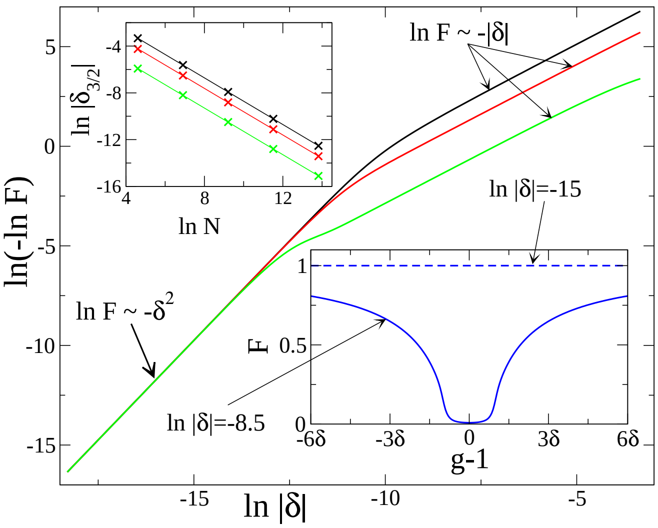

FIG. 2: (color online) Transition in the Ising chain from analytic to non-analytic regime as a function of parameter difference δ at fixed system size $N = 10^5$. The curves from top to bottom correspond to $\mathcal{F}(1, \delta)$, $\mathcal{F}(1 + \delta, \delta)$ and $\mathcal{F}(1 + 5\delta, \delta)$ (1). As we go from small to large δ's the slope of the curves changes smoothly from 2 to 1. The crossover region between the two limits is at $|\delta| = |\delta_{3/2}|$ where the slope equals 3/2. To numerically locate it, we have calculated $\mathcal{F}(1, \delta)$, $\mathcal{F}(1 + \delta, \delta)$ and $\mathcal{F}(1 + 5\delta, \delta)$ – as in the main figure – for various N's and found that the crossover condition is reached for $N|\delta_{3/2}| \sim 1$. This is illustrated in the upper inset where the power-law fits (straight lines) to numerical data (crosses) give $|\delta_{3/2}| = (0.2 \div 1.4)/N^{0.996\pm0.002}$. Order of the curves in the upper inset is the same as on the main plot. Lower inset shows that fidelity stays close to unity for small δ's (dashed line calculated for $\ln|\delta| = -15$) and explores all the values between zero and unity when parameter difference increases (solid line calculated for $\ln|\delta| = -8.5$). Difference between our theory, Eq. (4), and the latter numerical result (not shown in the inset) is *barely* visible on the scales explored in the lower inset.

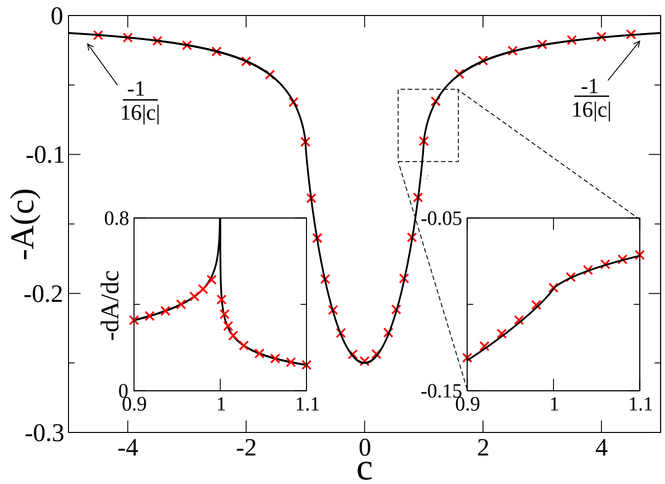

FIG. 3: (color online) Scaling function $A(c)$ of the Ising chain: see (4) and (5). Right inset highlights singularity at $c = 1$ point, while the left one presents the logarithmic divergence of $dA/dc|_{c=1}$ discussed in the text. The solid black lines provide the analytic description (5). The red crosses illustrate that numerics, obtained for $N = 10^5$ and $\delta = \pi 10^{-3}$, closely follows our theory.

Second, Eq. (4) 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 $\mathcal{F}(1, \delta) = \exp(-N|\delta|/4)$, but if one of the ground states is obtained at the critical point, $\mathcal{F}(1 \pm \delta, \delta) = \exp(-N|\delta|(\pi-2)/4\pi)$. In the opposite limit of $N|\delta| \ll 1$, $\mathcal{F} \approx 1 - \delta^2 N^2/16$ in both cases explaining the collapse of all curves in this limit in Figs. 1 and 2.

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 $N \to \infty$ such that $N|\delta| \gg 1$. This reflects singularity of the wave-function at the critical point approached in the thermodynamic limit. Quantitatively, $dA(c)/dc|_{c\to1^\pm} = \ln|1-c|/4\pi - 3\ln 2/4\pi + (1 \pm 1)/8 + \mathcal{O}((1-c)\ln|1-c|)$, which is logarithmically divergent at $c = 1$ (Fig. 3). This divergence is a signature of a pinch point found in [15, 18, 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 (4) a compact expression for fidelity away from the critical point. Taking $|c| \gg 1$ (but still $|\epsilon| \ll 1$), $A(c) \simeq 1/16|c|$ and so

$$\mathcal{F} \simeq \exp(-N\delta^2/16|\epsilon|). \quad (6)$$

This reduces to a known result for fidelity susceptibility when the argument of the exponent is small and so $\mathcal{F} \approx 1 - \delta^2 N/16|\epsilon|$ (see e.g. [9]), but provides a new result in the opposite limit where lowest order Taylor expansion is insufficient. We notice also that (6) is analytical in δ even in the limit of $N \to \infty$, which is in agreement with our intuition: there are no singularities expected when the system is far away from the critical point.

All the above results can be generally derived by studying the so-called scaling parameter

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

introduced in [18] in the context of fidelity per site approach to the thermodynamic limit. We expect that this limit is reached when

$$\min[(\xi(g + \delta), \xi(g - \delta)] \ll L, \quad (7)$$

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 (7) is equivalent to $L|\delta|^\nu \gg 1$ [22]. For the Ising chain studied above it reads $N|\delta| \gg 1$ properly predicting the crossover condition numerically found: see (3) and Figs. 1 and 2.

Generalizing the scaling theory of second order QPTs (Sec. 1.4 of [23]), 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 get $\tilde{d}(g + \delta, g - \delta) = |\delta|^{d\nu} f(c + 1, c - 1)$, which for constant c gives

$$\ln \mathcal{F} \sim -N|\delta|^{d\nu}, \tag{8}$$

in agreement with Ising chain calculation (4) for which $f(c+1, c-1)$ equals $A(c)$. In a general context, Eq. (8) shows how universal part of the scaling parameter causes the Anderson catastrophe near a critical point.

We assume below $\epsilon, \delta > 0$ for simplicity and set b through $(\epsilon + \delta)b^{1/\nu} = 1$ to expand the scaling function f away from the critical point ($\delta \ll \epsilon \ll 1$). 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

$$\ln \mathcal{F} \sim -N\delta^2|\epsilon|^{d\nu-2}. \tag{9}$$

When the system is small enough, $N\delta^2|\epsilon|^{d\nu-2} \ll 1$, but still in the thermodynamic limit (7), we reproduce the known result for fidelity susceptibility $1-\mathcal{F} \sim \delta^2 N|\epsilon|^{d\nu-2}$ [11, 16]. Otherwise, Eq. (9) provides a new result again in agreement with the Ising model calculation (6).

To check our scaling predictions in a system belonging to another universality class, we have studied the extended Ising model [14, 18, 24] where $z = 2$ and $\nu = 1$. It also supports Eqs. (8) and (9) [25]. 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, which requires further investigation [25].

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 fidelity have been already done [26, 27].

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. Gu, ArXiv e-prints (2008), 0811.3127.
[10] J. Dziarmaga, eprint, arXiv:0912.4034 (to appear in Advances in Physics).
[11] R. A. Barankov, ArXiv e-prints (2009), 0910.0255.
[12] V. Gritsev and A. Polkovnikov, ArXiv e-prints (2009), 0910.3692.
[13] B. Damski, H. T. Quan, and W. H. Zurek, ArXiv e-prints (2009), 0911.5729.
[14] M. Cozzini, R. Ionicioiu, and P. Zanardi, Phys. Rev. B **76**, 104420 (2007).
[15] H. Zhou, R. Orús, and G. Vidal, Phys. Rev. Lett. **100**, 080601 (2008).
[16] A. F. Albuquerque, F. Alet, C. Sire, and S. Capponi, Phys. Rev. B **81**, 064418 (2010).
[17] W.-L. You, Y.-W. Li, and S.-J. Gu, Phys. Rev. E **76**, 022101 (2007).
[18] H. Zhou and J. P. Barjaktarevič, J. Phys. A **41**, 412001 (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 as in Fig. 2. If this is the case, the system *approaches* the non-analytic limit.
[21] P. W. Anderson, Phys. Rev. Lett. **18**, 1049 (1967).
[22] The opposite limit, $L|\delta|^\nu \ll 1$, provides a condition for validity of the fidelity susceptibility approach near a critical point (see e.g. [11]).
[23] M. A. Continentino, *Quantum Scaling in Many-Body Systems* (World Scientific Publishing, Singapore, 2001).
[24] M. M. Wolf, G. Ortiz, F. Verstraete, and J. I. Cirac, Phys. Rev. Lett. **97**, 110403 (2006).
[25] M.M. Rams and B. Damski, *in preparation*.
[26] J. Zhang, X. Peng, N. Rajendran, and D. Suter, Phys. Rev. Lett. **100**, 100501 (2008).
[27] J. Zhang *et al.*, Phys. Rev. A **79**, 012305 (2009).