Negativity as the entanglement measure to probe the Kondo regime in the spin-chain Kondo model

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We study the entanglement of an impurity at one end of a spin chain with a block of spins using negativity as a true measure of entanglement to characterize the unique features of the gapless Kondo regime in the spin-chain Kondo model. For this spin chain in the Kondo regime we determine—with a true entanglement measure—the spatial extent of the Kondo screening cloud, we propose an ansatz for its ground state and demonstrate that the impurity spin is indeed maximally entangled with the cloud. To better evidence the peculiarities of the Kondo regime, we carry a parallel analysis of the entanglement properties of the Kondo spin-chain model in the gapped dimerized regime. Our study shows how a genuine entanglement measure stemming from quantum information theory can fully characterize also nonperturbative regimes accessible to certain condensed matter systems.

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I. INTRODUCTION

The investigation of entanglement or the truly "quantum" correlations inherent in many-body condensed matter systems is currently a topic of intense activity.[1–9] This emerging area aims at characterizing many-body states using tools and measures developed in quantum information. Till date, most investigations have focused on either the entanglement between individual elements, such as single spins, or the entanglement between two complementary blocks of a many-body system. The former entanglement is generically nonzero only between nearest or next to nearest neighbors.[2,3] For complementary blocks, the whole system is in a *pure state* and the von Neumann entropy is a *permissible* measure of the entanglement. In this context much interest has been evoked by conventional gapless phases, where, due to the absence of an intrinsic length scale, the von Neumann entropy diverges with the size of the blocks.[4–6] In this backdrop, it is timely to investigate the entanglement in gapless regimes of a many-body system for which its true form and amount may not be characterized through the entanglement between individual spins or complementary blocks. Kondo systems are ideal candidate for these investigations.[7,10]

Kondo systems[7,10] are expected to be very distinctive in the context of entanglement for at least two reasons, (i) Despite being "gapless," they support the emergence of a length scale ξ, the so called Kondo screening length,[7,10]which should be reflected in the entanglement, making it markedly different from that in the more conventional gapless models studied so far; (ii) They are expected to have a more exotic *form* of entanglement than the widely studied spin-spin and complementary block entanglements. Indeed, in Kondo systems, the impurity spin is expected to be mostly entangled with only a specific block of the whole system. This is, of course, merely an intuition which needs to be quantitatively verified with a genuine measure of entanglement: this is indeed the task accomplished in this paper, where we provide the only characterization of the Kondo regime based entirely on a true measure of entanglement.

The simplest Kondo model[10,11] describes a single impurity spin interacting with the conduction electrons in a metal; the ground state is a highly nontrivial many body state in which the impurity spin is screened by conduction electrons in a large orbital of size ξ. Many physical observables vary on the characteristic length scale ξ, which is a well defined function of the Kondo coupling.[10] Determining the spatial extent of the Kondo cloud has been so far a challenging problem repeatedly addressed by various means.[7,12,13] This includes an investigation which introduces a quantity called "impurity entanglement entropy″ which, however, is not a measure of entanglement and cannot *quantify* the entanglement within the system.[7,8] Recently,[14] it has been pointed out that the universal low energy long distance physics of this Kondo model arises also in a spin chain when a magnetic impurity is coupled to the end of a gapless Heisenberg antiferromagnetic J_1-J_2 spin 1/2 chain, where J_1 (J_2) is the (next) nearest-neighbor coupling. When J_2 exceeds a critical value, the spin chain enters a gapped dimerized regime and its relation to the Kondo model breaks down. Namely, for $0 \le J_2 \le J_2^c = 0.2412$, the spin system is gapless and it supports a Kondo regime.[7,8] For $J_2 > J_2^c$, the system enters the gapped *dimer regime*, where the ground state takes a dimerized form; at the Majumdar–Ghosh[15] point $(J_2 = 0.5)$, the ground state becomes just a tensor product of singlets. For $J_2 > 0.5$, incommensurability effects[16] emerge.

Our aim in this paper is to use a true measure of entanglement to fully characterize the unique features of the gapless Kondo regime in the spin chain Kondo model. Namely, for this spin chain in the Kondo regime: (i) we demonstrate that the impurity spin is indeed maximally entangled with the Kondo cloud; (ii) we determine the spatial extent of the Kondo screening length ξ using only an entanglement measure; (iii) we motivate an ansatz for its ground state in the Kondo regime; (iv) we evidence the scaling of a true measure of entanglement as pertinent parameters are varied. In order to accomplish these tasks we device a density matrix renormalization group (DMRG) approach enabling to investigate the entanglement between a single spin and a pertinent

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block of the chain, which may be applied in other contexts. Finally, to better evidence the unique properties of the entanglement in the Kondo regime we carry a parallel analysis of the entanglement properties of this model in the gapped dimerized regime. Using a true measure of entanglement to determine ξ enables to exploit the peculiarities of the Kondo regime of a spin chain to generate long-range distance independent entanglement usable for quantum communication tasks.[17]

A true measure of entanglement should satisfy a set of postulates, for example, it should be nonincreasing under local actions, such a genuine measure does exist for two subsystems of arbitrary size even when their combined state is mixed, as it happens in Kondo systems. This measure is the *negativity*[18] and it has been successfully used to quantify the entanglement in a harmonic chain[19,20] and between distant regions of critical systems.[21,22] For bipartite systems, negativity is defined as $E=\Sigma_i|a_i|-1$, where a_i denote the eigenvalues of the partial transpose of the whole density matrix of the system with respect to one of the two subsets of the given partition and $|\ldots|$ is the absolute value.[18]

The paper is organized as follows: In Sec. II, we define an entanglement healing length for the spin chain Kondo model; Sec. III explains the DMRG-based approach we devised in order to compute its entanglement properties. In Sec. IV, we show the remarkable scaling of a true measure of entanglement (i.e., negativity) in the Kondo regime attainable by the Kondo spin chain when $0 \le J_2 \le J_2^c = 0.2412$; in addition, we motivate an ansatz for the ground state of this chain in the Kondo regime. Section V is devoted to a summary of our results and to a few concluding remarks.

II. MEASURING THE ENTANGLEMENT HEALING LENGTH

The spin chain Kondo model[14] is defined by the Hamiltonian,

$$H = J'(\sigma_1 \,.\, \sigma_2 + J_2 \sigma_1 \,.\, \sigma_3) + \sum_{i=2}^{N-1} \sigma_i \,.\, \sigma_{i+1} + J_2 \sum_{i=2}^{N-2} \sigma_i \,.\, \sigma_{i+2}, \tag{1}$$

where $\sigma_i = (\sigma_i^x, \sigma_i^y, \sigma_i^z)$ is a vector of Pauli operators at site i, N is the total length of the chain, J_2 is the next nearest neighbor coupling and the nearest neighbor coupling J_1 has been normalized to 1. The impurity spin, located at one end of the chain, is accounted for by weaker couplings to the rest of the system; in the following, see Fig. 1(a), both couplings J_1 and J_2 are weakened by the same factor J', which quantifies then the impurity strength.

To study the entanglement of the ground state we divide [see Fig. 1(b)] all the spins of the chain in three different groups, the impurity spin, block A, which contains the L spins next to the impurity ($L=0,1,\ldots,N-1$) and block B formed by the remaining $N-L-1$ spins. We use negativity to fully characterize the entanglement between the impurity and block B in both the gapless Kondo and the gapped dimerized regimes. We determine the size of the block A when the entanglement between the impurity and block B is almost zero; by this procedure we measure an entanglement healing length (EHL) L^*, i.e., the length of the block A which is maximally entangled with the impurity. We show that, in the gapless Kondo regime, EHL scales with the strength of the impurity coupling just as the Kondo screening length, ξ, does. Thus, in the gapless regime of the Kondo spin chain, our approach yields a method to detect the Kondo screening length[7,12,13] based on a true measure of entanglement. In addition, we *find* that entanglement, as quantified by negativity, is a homogeneous function of two ratios: N/L^* and L/N, where L is the size of the block A, i.e., the block adjacent to the impurity, and N is the length of the whole chain. As a result, the entanglement in the Kondo regime is essentially unchanged if one rescales all the length scales with the EHL L^*.

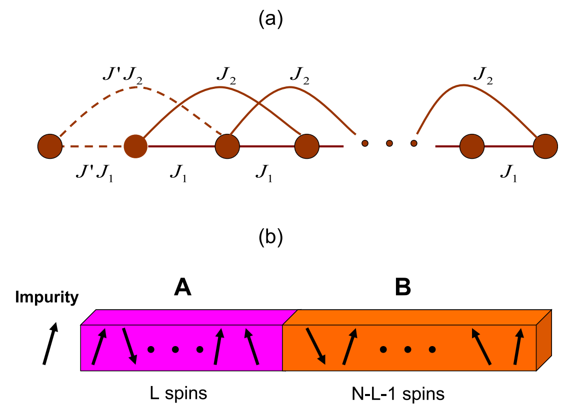

FIG. 1. (Color online) (a) Kondo Spin chain with next nearest neighbor Heisenberg interaction with one impurity at one end. (b) The chain is divided into three parts, an impurity, a block A and a block B. Entanglement is computed between the impurity and block B.

III. DMRG ANALYSIS OF ENTANGLEMENT IN THE SPIN-CHAIN KONDO MODEL

We use the DMRG[23] approach to compute the ground state of the spin chain Kondo model. We analyze large chains, $N=250$, to avoid finite size effects and take N to be even to avoid problems arising from accidental degeneracies. In a DMRG approach the ground state of the system is partitioned in terms of states of a left block, a right block (not to be confused with blocks A and B) and two intermediate spins as shown in Fig. 2(a). The states of the intermediate spins are given in the computational ($|\uparrow\rangle, |\downarrow\rangle$) basis, while the states of the both blocks are usually in some non-trivial truncated DMRG basis. In this approach one has several representations for the ground state which vary due to the number of spins in the left (right) block and it is possible to go from one representation to the other by applying pertinent operators on each block. The main issue in the DMRG is that the dimension of the left (right) block is kept constant independent of whatever spins are there in that block. To have a fixed dimension for the left (right) block we truncate the Hilbert space such that the amount of entanglement between the two parts of the chain remains almost unchanged.[23] To have a

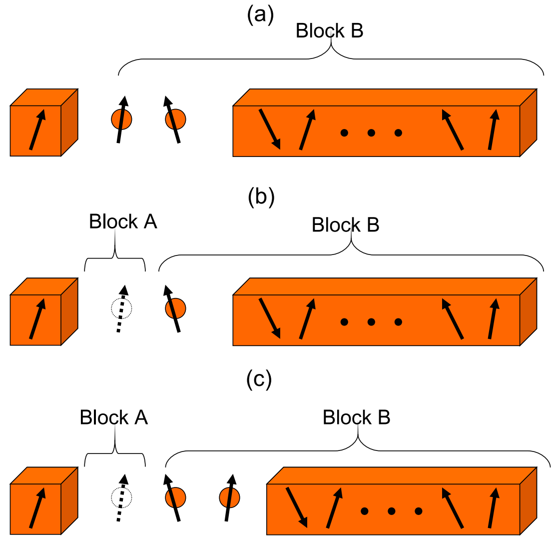

FIG. 2. (Color online) (a) DMRG representation of the state of the chain keeps two intermediate spins in ordinary computational basis and the left and right blocks in a truncated DMRG basis. (b) The intermediate spin next to the impurity is traced out from the density matrix of the chain. This tracing is equivalent to adding the traced out spin to block A. (c) The basis of the right block of DMRG representation is transformed so that a single spin in the left side of the right block is represented in the computational basis while the state of the new right block is given in a DMRG basis.

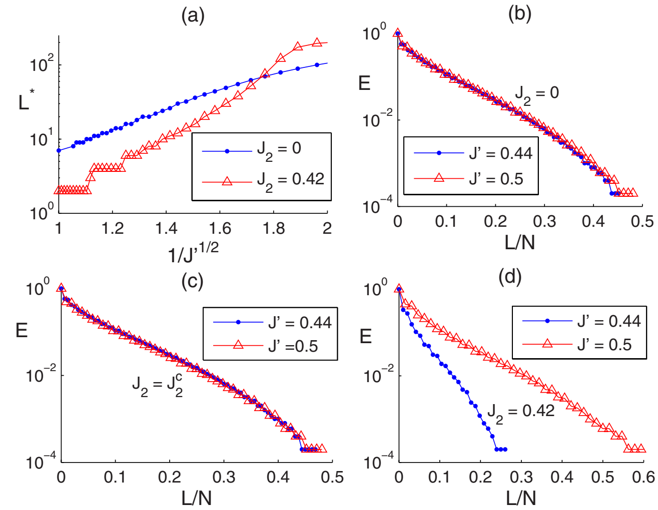

FIG. 3. (Color online) (a) L^* vs $1/\sqrt{J'}$ for both Kondo (J_2=0) and dimer regime (J_2=0.42). (b) Entanglement vs L/N for fixed N/L^*=4 when J_2=0. (c) Entanglement vs L/N for fixed N/L^*=4 at the critical point J_2=J_2^c. (d) Entanglement vs L/N for fixed N/L^*=4 in the dimer regime (J_2=0.42).

precise results we need to sweep all representations of the ground state for several times to get the proper basis for the left and the right blocks of all representations. After some sweeps, when the ground-state energy converges (we keep states for which the error of the energy would be less than 10^{-6}), we pause to compute the entanglement. We take a representation of the ground state, in which the left block contains just the single impurity spin and the right block contains $N-3$ spins: as a result, the single impurity spin is given in the computational basis and this allows us to compute the negativity later. From this DMRG state, we trace out the spins belonging to block A before computing the entanglement between the impurity and block B since it is most convenient to compute the entanglement between the impurity and the block B: due to the entanglement monogamy, this provides an equivalent information about the entanglement of the impurity with the block A. Our tracing procedure starts with the density matrix of the ground state of the system in the representation shown in Fig. 2(a); at this stage, the number of spins in the block A is zero (no spin has been traced out), all spins except the impurity belong to the block B, and the entanglement between the impurity and the block B is maximal (i.e., E=1). Then, we trace out the intermediate spin next to the impurity as shown in Fig. 2(b); this amounts to putting that spin into block A. Finally, as shown in Fig. 2(c), we transform the DMRG basis of the right block so as to put a single spin at the left of the right block in the computational basis, while the state of the new right block is given in a DMRG basis. As a consequence, the resulting density matrix has the exact form of Fig. 2(a) and we can continue the procedure to trace one spin at each step (i.e., put more spins in the block A) and compute the entanglement between impurity and block B.

IV. SCALING OF NEGATIVITY AND ANSATZ FOR THE GROUND STATE IN THE KONDO REGIME

We find that there is an EHL L^* so that, for $L>L^*$, the entanglement between the impurity and block B is almost zero: L^* provides us with an estimate of the distance for which the impurity is mostly entangled with the spins contained in block A. For large chains ($N>200$) in the Kondo regime, one finds that L^* is almost independent of N and depends only on J'. In the Kondo regime, i.e. for $J_2<J_2^c$, L^* depends on J' just as the Kondo screening length ξ does;[7,8] for small J', $L^*\propto e^{\alpha/\sqrt{J'}}$, where α is a constant. We plot L^* as a function of $1/\sqrt{J'}$ in Fig. 3(a). In a semilogarithmic scale, the straight line plot exhibited in the Kondo regime (J_2=0) shows that L^* may be regarded as the Kondo screening length. Moreover, the nonlinearity of the same plot in the dimer regime (J_2=0.42), especially for small J', shows that, here, no exponential dependence on $1/\sqrt{J'}$ holds.

We observe also a remarkable scaling of negativity in the Kondo regime. This scaling may be regarded as yet another independent evidence of the fact that L^* is indeed the Kondo length ξ. In general, the entanglement E between the impurity and block B is a function of the three independent variables, J', L and N which, due to the one to one correspondence between J' and L^*, can be written as $E(L^*,L,N)$. We find that, in the Kondo regime, $E=E(N/L^*,L/N)$. To illustrate this, we fix the ratio N/L^* and plot the entanglement in terms of L/N for different values of J' (or equivalently L^*) for J_2=0 [Fig. 3(b)] and for J_2=J_2^c [Fig. 3(c)]. The complete coincidence of the two plots in Figs. 3(b) and 3(c) shows that, in the Kondo regime, the spin chain can be scaled in size without essentially affecting the entanglement as long as L^* is also scaled. In the dimer regime the entanglement stays a function of three independent variables, i.e., E =$E(L^*,L,N)$, and, as shown in Fig. 3(d), the entanglement does not scale with L^*. In our approach, the Entanglement

Healing Length L^* may be evaluated in both the Kondo and the dimer regime: the scaling behavior, as well as the dependence of L^* on J', discriminates then between the very different entanglement properties exhibited by the spin chain Kondo model as J_2 crosses J_2^c.

We defined L^* such that there is no entanglement between the impurity and block B when block A is made of L^* spins. Conventional wisdom based on previous renormalization group analysis suggests that, in both regimes, the impurity and the block A of length L^* form a pure entangled state, while block B is also in a pure state. This is indeed approximately true in the dimer regime (exactly true for J_2=0.5) but it turns out to be dramatically different in the Kondo regime. To check this, we computed the von Neumann entropy of the block B when block A has L^* spins and found it to be nonzero. Thus, the blocks A and B are necessarily entangled in the Kondo regime as there is no entanglement between the impurity and B. In fact, after a distance L^*, the impurity is "screened," i.e., the block B feels as if it is part of a conventional gapless chain and has a diverging von Neumann entropy. The Kondo cloud is maximally entangled with the impurity as well as being significantly entangled with block B. Based on the above, a simple ansatz for the ground state $|GS\rangle$ in the Kondo regime is provided by

$$|GS\rangle = \sum_i \alpha_i \frac{|\uparrow\rangle|L_i^{\uparrow}(J')\rangle - |\downarrow\rangle|L_i^{\downarrow}(J')\rangle}{\sqrt{2}} \otimes |R_i(J')\rangle, \tag{2}$$

where α_i are constants, $\{|L_i^{\uparrow}(J')\rangle, |L_i^{\downarrow}(J')\rangle\}$ and $\{|R_i(J')\rangle\}$ are sets of orthogonal states on the cloud and the remaining system, respectively. At the fixed point $J' \to 0$ all spins except the impurity are included in $|L_i^{\uparrow}(J')\rangle$ and $|L_i^{\downarrow}(J')\rangle$. At $J' \to 1$, very few spins are contained in $|L_i^{\uparrow}(J')\rangle$ and $|L_i^{\downarrow}(J')\rangle$ while $\{|R_i(J')\rangle\}$ represents most of the chain.

For what concerns the mere evaluation of the amount of entanglement as J' is varied, we first plot, in Fig. 4(a), the negativity as a function of L near the two fixed points, i.e. $J' \to 0$ and $J' \to 1$, accessible in the Kondo regime: as expected, near $J' \to 0$ (i.e., for large values of the Kondo screening length), the entanglement remains large for rather large values of L while, for $J' \to 1$ (i.e., for a very small cloud) it decreases rapidly with L. Figure 4(a) (semilogarithmic) shows that, also at the extreme limits $J' \to 0$ and $J' \to 1$, the entanglement decays exponentially with L since this a characteristic mark of the entanglement in the Kondo regime. This exponential decay of entanglement is absent in the dimer regime, Fig. 4(b) shows that, here, only for rather large J', the entanglement decays exponentially with L while, for small J', the entanglement between the impurity and block B decays *slower than an exponential* as a function of L exhibiting even a plateau at short distances. This latter feature is evidenced in Fig. 4(c), and is consistent with the emergence, for small J', of long-range valence bonds between the impurity and far spins as a consequence of the onset of the dimerized ground state.[7] In fact, when J' is small, J_2J' becomes much less than J_2^c and the impurity forms valence bonds with distant spins, while the other spins, since for them $J_2 > J_2^c$, form a valence bond with their nearest neighbor to preserve the dimerized nature of the ground state: as a result, the impurity shares less entanglement with nearby spins and fulfills its capacity of entanglement forming valence bonds with the more distant spins in the chain.

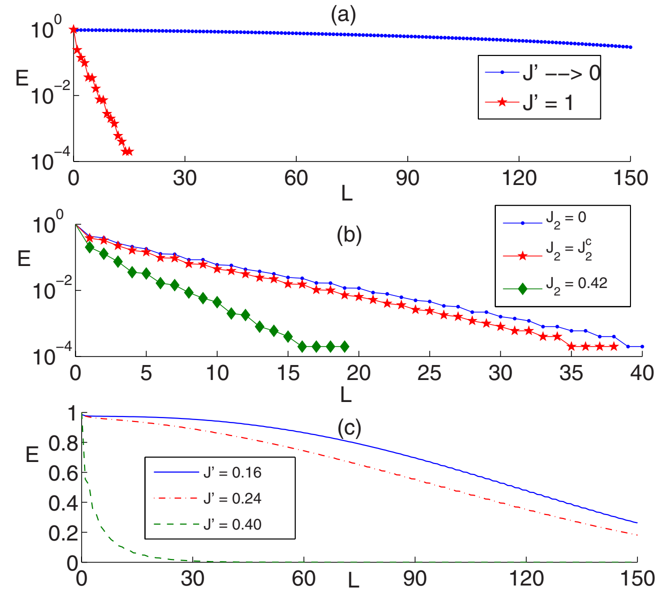

FIG. 4. (Color online) (a) Entanglement vs L for the two fixed points $J' \to 0$ and $J' \to 1$ in the Kondo regime J_2=0. (b) Exponential decay of entanglement in terms of L in a chain of length N =250 for J'=0.6. (c) Nonexponential decay for small J' in the dimer regime J_2=0.42.

V. SUMMARY AND CONCLUDING REMARKS

To summarize, we analyzed the Kondo spin chain model from the viewpoint of a genuine entanglement measure, namely the negativity. This readily shows that the impurity spin is indeed maximally entangled with the Kondo cloud. We used negativity to provide an *independent* method to determine the Kondo screening length and to provide a characterization of the ground state of the Kondo spin chain in the Kondo regime. We found that, not only is the Kondo regime of this model distinct from the gapless phases probed to date using the von Neumann entropy, but the form of the entanglement—a spin and a block in a mixed state—is also distinctive. We devised a DMRG approach enabling to compute the entanglement between the impurity and a block of spins located at the other side of the chain for different lengths of the block. We showed that, in the Kondo regime, the EHL L^* scales with the impurity coupling J' just as the Kondo length does: in other words, the impurity, though not entangled with any individual spin, is shown to be entangled with the totality of the spins within the Kondo cloud—whose size is measured by L^*—and disentangled from the rest. Our measure of the entanglement in the Kondo regime led us to formulate an ansatz for the ground state of the Kondo spin chain for $J_2 < J_2^c$. Our approach also shows that, in the Kondo regime, the entanglement scales exponentially with L/L^* and that, in the gapped dimer regime, though it is still possible to define an EHL, the impurity-block entanglement is usually smaller and has no characteristic length scale.

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[1] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).

[2] M. C. Arnesen, S. Bose, and V. Vedral, Phys. Rev. Lett. **87**, 017901 (2001).

[3] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002); T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).

[4] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).

[5] B. Q. Jin and V. E. Korepin, J. Stat. Phys. **116**, 79 (2004).

[6] P. Calabrese and J. Cardy, J. Stat. Mech.: Theory Exp. (2004) P06002.

[7] E. S. Sørensen, M. S. Chang, N. Laflorencie, and I. Affleck, J. Stat. Mech.: Theory Exp. (2007) P08003; (2007) L01001.

[8] N. Laflorencie, E. S. Sørensen, M. S. Chang, and I. Affleck, Phys. Rev. Lett. **96**, 100603 (2006).

[9] K. Le Hur, P. Doucet-Beaupre, and W. Hofstetter, Phys. Rev. Lett. **99**, 126801 (2007); K. Le Hur, Ann. Phys. **323**, 2208 (2008).

[10] I. Affleck, arXiv:0809.3474 (unpublished).

[11] A. Hewson, *The Kondo Model to Heavy Fermions* (Cambridge University, Cambridge, England, 1997).

[12] H. Frahm and A. A. Zvyagin, J. Phys.: Condens. Matter **9**, 9939 (1997).

[13] R. G. Pereira, N. Laflorencie, I. Affleck, and B. I. Halperin, Phys. Rev. B **77**, 125327 (2008).

[14] N. Laflorencie, E. S. Sorensen, and I. Affleck, J. Stat. Mech.: Theory Exp. (2008) P02007.

[15] C. K. Majumdar and D. K. Ghosh, J. Phys. C **3**, 911 (1970).

[16] U. Schollwock, Th. Jolicoeur, and T. Garel, Phys. Rev. B **53**, 3304 (1996).

[17] P. Sodano, A. Bayat, and S. Bose, arXiv:0811.2677 (unpublished).

[18] G. Vidal and R. F. Werner, Phys. Rev. A **65**, 032314 (2002); M. B. Plenio, Phys. Rev. Lett. **95**, 090503 (2005).

[19] K. Audenaert, J. Eisert, M. B. Plenio, and R. F. Werner, Phys. Rev. A **66**, 042327 (2002).

[20] J. Kofler, V. Vedral, M. S. Kim, and C. Brukner, Phys. Rev. A **73**, 052107 (2006).

[21] H. Wichterich, J. Molina-Vilaplana, and S. Bose, Phys. Rev. A **80**, 010304(R) (2009).

[22] S. Marcovitch, A. Retzker, M. B. Plenio, and B. Reznik, Phys. Rev. A **80**, 012325 (2009).

[23] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992); S. R. White, Phys. Rev. B **48**, 10345 (1993).