PHYSICAL REVIEW A **85**, 013645 (2012)

Quantum phase transition of two-mode Bose-Einstein condensates with an entanglement order parameter

Wei Fan,[1] Yan Xu,[1,2,*] Bing Chen,[1] Zhaoyang Chen,[3,†] Xunli Feng,[4] and C. H. Oh[4,‡]

[1]*College of Science, Shandong University of Science and Technology, Qingdao 266510, China*

[2]*Centre for Quantum Technologies, National University of Singapore, 3 Science Drive 2, Singapore 117543*

[3]*Department of Mechanical Engineering, University of California, Berkeley, California 94720, USA*

[4]*Center for Quantum Technologies and Physics Department, Faculty of Science, National University of Singapore, 2 Science Drive 3, Singapore 117542*

(Received 13 September 2011; published 31 January 2012)

The ground-state entanglement of the two-mode Bose-Einstein condensate is investigated through a quantum-phase-transition approach. The entanglement measure is taken as the order parameter and this is a nonlocal order parameter, which is different from the conventional order parameter of the Mott-insulator–superfluid-phase transitions. For this nonlocal order parameter, the scaling behavior corresponding to a continuous phase transition is obtained and a power-law divergence near the critical region follows it. This scaling behavior of quantum entanglement is analyzed by the finite-size scaling and the critical exponents are obtained as $\nu = 1.01$ and $\gamma = 0.86$. A close connection between quantum fluctuations and the phase transition of entanglement is also obtained.

DOI: 10.1103/PhysRevA.85.013645 PACS number(s): 03.75.Gg, 05.30.Rt

I. INTRODUCTION

Quantum entanglement is a key feature of quantum information theory and is one of the most active research areas in recent years [1], especially in combination with condensed-matter systems [2]. Beyond its generation and application, one of the essential questions is how to understand the process that occurs in a physical system when it transitions from nonentangled to entangled states. One approach to study this phenomenon is to treat it as a quantum phase transition, where the order parameter is the entanglement measure. This approach combines the theory of critical phenomenon with the theory of quantum information. For spin-lattice models, many results have been obtained. The concurrence [3,4] is often used as the entanglement measure in spin models. Entanglement exhibits scaling behavior near the critical region and the critical behavior is shown to be logarithmic [5–8]. The phase transition is second order for the ferromagnetic case and first order for the antiferromagnetic case [9].

While the critical behavior of quantum entanglement in spin models has widely been studied, there are very few studies on that in boson systems. It is thus of interest to investigate the critical behavior of quantum entanglement in boson systems.

One extensively studied boson system in quantum entanglement is the two-mode Bose-Einstein condensates coupled via Josephson tunneling [10]. It is described by the Hamiltonian [11]

$$\mathcal{H} = \frac{K}{8}(N_1 - N_2)^2 - \frac{\Delta\mu}{2}(N_1 - N_2) - \frac{\varepsilon_J}{2}(a_1^\dagger a_2 + a_2^\dagger a_1), \quad (1)$$

where a_1,a_2 are the annihilation operators for the two modes (1 and 2), respectively, and $N_1 = a_1^\dagger a_1, N_2 = a_2^\dagger a_2$ are the corresponding number operators. The parameter K provides the atom-atom interaction, $\Delta\mu$ is the difference in the chemical potential between the two modes, and ε_J is the coupling for tunneling. This Hamiltonian describes both the double-well Bose-Einstein condensate and the two-level Bose-Einstein condensate in a single potential. For the first case, the tunneling between the two wells must be small to use this Hamiltonian, while for the second case, there is no such restriction. We will show in this paper that the phase transition occurs at very small couplings, so the quantum-phase-transition approach can describe both cases. The entanglement production in this system has been extensively studied [10,12–15]. The von Neumann entropy [16] $E(\rho)$ is the usually used entanglement measure, where ρ is the density matrix of the system, and for a system size of N particles, the maximum entropy is $E_{\max} = \log_2(N+1)$.

This Hamiltonian (1) is, in fact, a two-site version of the Bose-Hubbard model [17]. When varying the ratio between the interaction term and the coupling term through a critical value, a quantum phase transition occurs in the Bose-Hubbard model, which is the Mott-insulator to the superfluid transition [18]. This phase transition is driven by quantum fluctuations and the order parameter is the conventional wave function. In the Mott-insulator phase, atoms are localized in lattice sites, while in the superfluid phase, atoms spread out over the whole system. Although the insulator-superfluid phase transition is studied extensively [19–23] both in theory and in experiment, it is interesting to investigate what would happen to the Bose-Hubbard model when taking a nonlocal order parameter, rather than the conventional order parameter.

In this paper, we present such a study for the simplest two-site Bose-Hubbard system, i.e., the two-mode Bose-Einstein condensate. The entanglement measure, namely, the von Neumann entropy, is taken as the nonlocal order parameter. We show that there is a critical point and entanglement exhibits scaling behavior near the critical point, which can be analyzed using the theory of critical phenomena. We

*x1y5hot@gmail.com
†zychen@berkeley.edu
‡phyohch@nus.edu.sg

identify this as a continuous phase transition. This phase transition is different from the insulator-superfluid phase transition because it is obtained for a nonlocal order parameter, rather than the conventional order parameter. The critical behavior of quantum entanglement is shown to be power-law divergent, which is different from the logarithmic divergence of spin-lattice models. Our work may improve the combination of methods in critical phenomena and quantum information theory for the boson systems, especially for the Bose-Hubbard model. A further extension of this work is to investigate quantum phase transitions in the Bose-Hubbard model of dozens of lattice sites, where a new entanglement measure is also needed to be derived.

II. CONTINUOUS PHASE TRANSITION

In this paper, we only consider the case $K > 0$, which corresponds to a repulsive interaction between atoms. The total particle number is conserved and we set $\Delta\mu = 0$. By using the angular momentum operators

$$J_z = \tfrac{1}{2}(N_2 - N_1),$$
$$J_x = \tfrac{1}{2}(a_1^\dagger a_2 + a_2^\dagger a_1),$$
$$J_y = \tfrac{i}{2}(a_1^\dagger a_2 - a_2^\dagger a_1),$$

and neglecting constant terms, the Hamiltonian (1) is rewritten as

$$\mathcal{H} = \chi J_z^2 - \Omega J_x, \tag{2}$$

where $\chi = K/2$ and $\Omega = \varepsilon_J$. As we are only interested in the ratio between the two competing energy terms, it is convenient to introduce the dimensionless parameter Ω/χ in the calculation, so the Hamiltonian can be reduced to

$$\mathcal{H} = J_z^2 - \Omega J_x, \tag{3}$$

where we have redefined Ω using the dimensionless parameter, i.e., $\Omega/\chi \rightarrow \Omega$. This dimensionless coupling parameter can be viewed as an "external field" by analogy with Ising models. We also define the dimensionless entropy $E(\rho)/E_{\max} \rightarrow E(\rho)$ to make it easier to compare the results of different system sizes. We use numerical diagonalization to calculate [24,25] the ground-state entanglement and its susceptibility with respect to the external field Ω.

We first calculate the susceptibility $\frac{dE(\rho)}{d\Omega}$ with respect to the coupling Ω for various system sizes, which is shown in Fig. 1. We see that there is a critical point Ω_m for each system size, where the susceptibility reaches its critical value $\frac{dE(\rho)}{d\Omega}_m$. The critical susceptibility $\frac{dE(\rho)}{d\Omega}_m$ increases with the system size and would be divergent for an infinite system size that corresponds to the thermodynamic limit, which implies that this is a continuous phase transition where there is no discontinuity in the order parameter, as depicted by the inset for the system of $N = 2700$ particles. This will be verified further in Sec. IV.

From Fig. 1, the critical point Ω_m lies in the small coupling regime, which means the phase transition occurs shortly after the external field is switched on. We could easily figure that the critical value is $\Omega_c = 0$ for an infinite system size of the thermodynamic limit. When $\Omega = 0$, the Neumann entropy is zero and there is no two-mode entanglement in the system;

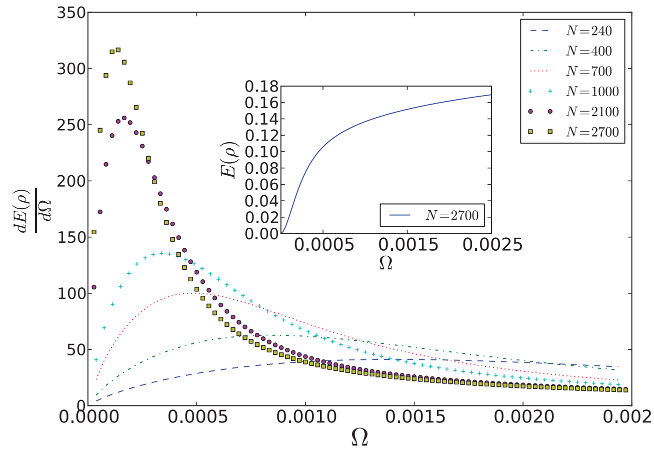

FIG. 1. (Color online) The susceptibility $\frac{dE(\rho)}{d\Omega}$ of the quantum entanglement with respect to the external field Ω for system sizes of $N = 240$, 400, 700, 1000, 2100, and 2700. A continuous phase transition occurs as the susceptibility diverges with the system size. The critical point Ω_m where the susceptibility attains its maximum $\frac{dE(\rho)}{d\Omega}_m$ lies in the Fock regime, and this critical susceptibility diverges with the system size. The inset depicts the change of the order parameter—the ground-state entanglement for the system of $N = 2700$, which increases continuously from zero. We choose even particle numbers because for odd particle numbers there is a degeneracy of the ground state when $\Omega = 0$.

when $\Omega > 0$, the Neumann entropy gets a finite value and entanglement is generated in the system. That means the system transitions from nonentangled to entangled states, i.e., two essentially different states, once Ω is switched on from 0, so the critical value is just 0. This will be verified further in Sec. III, where we numerically fit the critical point and the critical susceptibility for various system sizes. The critical point Ω_m is well fitted to N by choosing $\Omega_c = 0$.

III. POWER-LAW DIVERGENCE

The well-behaved relationship between the critical point and the system size in Fig. 2 is not just a coincidence. Actually it manifests the scaling behavior of quantum entanglement for this quantum system, which is typical in critical phenomenon. From Fig. 2, we obtain the scaling relationship

$$\Omega_m = 0.319225 N^{-0.989062} \tag{4}$$

for the critical point, and the scaling relationship

$$\frac{dE(\rho)}{d\Omega}_m = 0.393037 N^{0.846662} \tag{5}$$

for the critical susceptibility. The scaling behavior of the susceptibility is power-law divergent, in contrast to the logarithmic divergence of spin-lattice systems [5].

This power-law divergence of the susceptibility can be understood in the thermodynamic limit using a simple analysis. The basic idea is to truncate the Fock space of the system to just three basis states and use them to approximate the state of the system. The validity of this approximation lies in the fact that the critical point is $\Omega_c = 0$ and the delocalization process is very weak near this critical point, which means that the transitions between different basis states of the original Fock

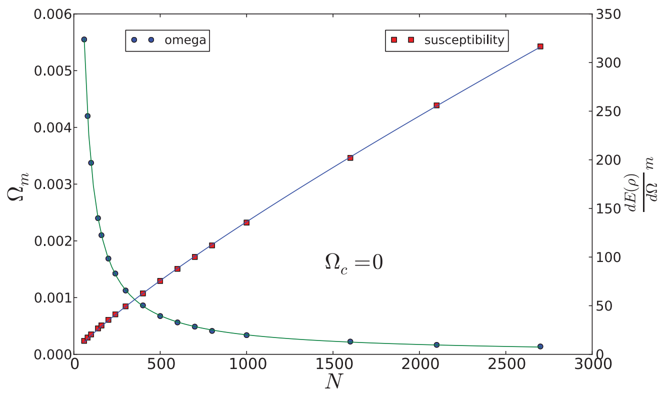

FIG. 2. (Color online) The scaling behavior of the quantum phase transition with the critical value $\Omega_c = 0$. The critical point Ω_m approaches 0 asymptotically by $\Omega_m \sim N^{-0.989062}$ and the susceptibility diverges in a power-law behavior captured by $\frac{dE(\rho)}{d\Omega}\big|_m \sim N^{0.846662}$, which is different from the logarithmic divergence of spin-lattice models.

space are very weak and we can use the three most important basis states for approximation. This is verified at the end of the calculation in Eq. (6), where a power-law behavior of the susceptibility is obtained and the divergent exponent does not differ much from that of the numerical simulation.

We choose the Fock space basis $|N_1, N_2\rangle$ for the system, where N_1 is the particle number on the first site and N_2 is the particle number on the second site. When $\Omega = 0$, the ground state is $|N/2, N/2\rangle$ with energy $E = 0$, that is, the system is in a self-trapping state without particle tunneling between the two sites. As Ω increases, the particles begin tunneling between the two sites and this delocalization process connects different basis states, so the system is described by $\sum_{n=0}^{N} c_n |n, N-n\rangle$. The critical value is $\Omega_c = 0$ and the delocalization process is very weak near this region, so we can truncate the Fock space of the system to just three basis states, i.e., $|N/2, N/2\rangle$, $|N/2-1, N/2+1\rangle$, and $|N/2+1, N/2-1\rangle$, then the state of the system is $|\psi\rangle = c_0|N/2, N/2\rangle + c_1|N/2-1, N/2+1\rangle + c_2|N/2+1, N/2-1\rangle$, where we assume the coefficient c_i to be real numbers for simplicity. As the probabilities of tunneling between the two sites are equal, the coefficients c_1 and c_2 are equal. By combining with the normalization condition $c_0^2 + c_1^2 + c_2^2 = 1$, we get the relationship $c_0 = \sqrt{1 - 2c_1^2}$. We next calculate the approximate ground state to determine the value of the coefficients,

$$\mathcal{H}|\psi\rangle = -\frac{\Omega N}{2} c_1 \left\{ \left| \frac{N}{2}, \frac{N}{2} \right\rangle + \frac{-\frac{\Omega N}{4}\sqrt{1-2c_1^2} + c_1}{-\frac{\Omega N}{2} c_1} \times \left[\left| \frac{N}{2} - 1, \frac{N}{2} + 1 \right\rangle + \left| \frac{N}{2} + 1, \frac{N}{2} - 1 \right\rangle \right] \right\} = E|\psi\rangle,$$

where the approximation $\sqrt{N/2(N/2+1)} \sim N/2$ is taken. The critical point $\Omega_c = 0$ determines that c_1 is a small number. From $|\psi\rangle = c_0[|N/2, N/2\rangle + c_1/c_0(|N/2-1, N/2+1\rangle + |N/2+1, N/2-1\rangle)]$, we obtain

$$E = -\frac{\Omega N}{2} \frac{c_1}{c_0},$$

which is approximately zero and is the ground-state energy near $\Omega_c = 0$, and

$$\frac{-\frac{\Omega N}{4}\sqrt{1-2c_1^2} + c_1}{-\frac{\Omega N}{2} c_1} = \frac{c_1}{\sqrt{1-2c_1^2}},$$

which gives the value

$$c_1^2 = \frac{1}{4}\left(1 - \frac{1}{\sqrt{1 + \frac{\Omega^2 N^2}{2}}}\right).$$

There are two values of c_1^2 and we choose the smaller one. Substituting the values of the coefficients into the von Neumann entropy,

$$E(\rho) = -c_0^2 \log_2 c_0^2 - c_1^2 \log_2 c_1^2 - c_2^2 \log_2 c_2^2,$$

and taking its derivative with respect to Ω gives

$$\frac{dE(\rho)}{d\Omega} \sim \frac{\Omega N^2}{\Omega^4 N^4} \sim N^{0.97}, \tag{6}$$

where the relationship $\Omega N \sim N^{0.01}$ from Eq. (4) in the thermodynamic limit is used. Thus we briefly illustrate the power-law divergence of the susceptibility in the thermodynamic limit.

The divergent exponent obtained in the analytic calculation is 0.97 and it is different from the value 0.85 of the numerical simulation in Eq. (5). This difference may be accounted for by the finite-size effects and the truncation errors. First, the analytic calculation manifests the thermodynamic limit, where there is no finite-size effect. The numerical result, however, is influenced by the finite-size effects, so this may be one of the reasons for the difference between the divergent exponents. Second, we adopt approximation in the analytic calculation by truncating the Fock space of the system to just three basis states. The numerical simulation, however, includes the full Fock space. The neglected basis states would certainly contribute to the result, although their amplitudes are small near the critical point. So the difference between the divergent exponent is also influenced by the truncation errors.

IV. FINITE-SIZE SCALING

A key feature of the critical phenomenon is the finite-size scaling. Phase transitions only occur at the thermodynamic limit, while numerical simulations can only deal with finite system sizes. To extract information from the results obtained from the finite system, finite-size scaling is required, where the effects of finite system sizes are eliminated by collecting all of the data of various system sizes onto a single curve and deducing the critical exponent in this process. In the phase transition of thermal order parameters, e.g., the magnetization, the critical exponent ν of the correlation length satisfies $|T - T_c| \sim N^{-1/\nu}$. By analogy, we obtain $\nu = 1/0.989062 \sim 1.01$ from Eq. (4), which is the critical exponent for the quantum phase transition of quantum entanglement. This critical exponent gives the reduced coordinate $N^{\nu}(\Omega - \Omega_m)$ for all of the finite system sizes. From Eq. (5), the susceptibility is reduced to $N^{-0.85}[\frac{dE(\rho)}{d\Omega} - \frac{dE(\rho)}{d\Omega}\big|_m]$. If the quantum entanglement of this model manifests quantum phase transitions, then all of the

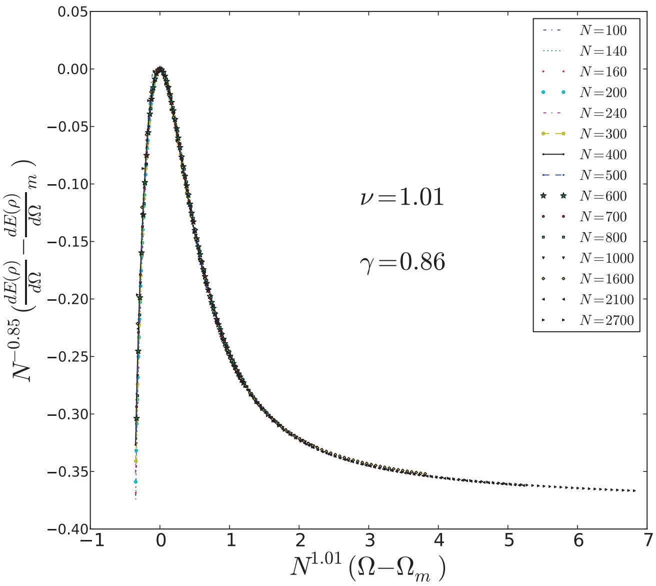

FIG. 3. (Color online) The finite-size scaling for the quantum phase transition of quantum entanglement. After the susceptibility is reduced by the system size to $N^{-0.85}[\frac{dE(\rho)}{d\Omega} - \frac{dE(\rho)}{d\Omega}_m]$, it becomes a function of $N^{1.01}(\Omega - \Omega_m)$. Data from a broad range of system sizes are collected on this single curve. The critical exponents obtained are $\nu = 1.01$ and $\gamma = 0.86$.

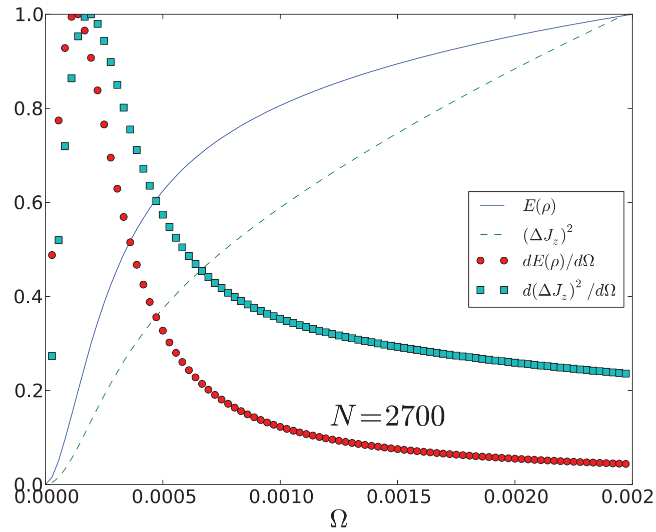

FIG. 4. (Color online) Comparison between $(\Delta J_z)^2$, $E(\rho)$ and their derivatives with respect to Ω. Their values are reduced to 1 by their maximum values. The increase of the quantum fluctuation corresponds to the increase of the order parameter, which indicates its connection with the phase transition of entanglement. There is a small "delay" between the derivative of the fluctuation and the susceptibility, with the susceptibility obtaining maximum value first. This delay comes from the finite-size effects.

data of various system sizes could be collected onto a single curve using the above reduced coordinates. This is indeed the case, as exhibited in Fig. 3. Again, this relationship is not just a coincidence. It illustrates that quantum entanglement of this model indeed belongs to a critical phenomenon. By resorting to the phase transition of the magnetization, where the susceptibility χ of the magnetization is reduced to $N^{-\gamma/\nu}\chi$, we obtain the critical exponent $\gamma = 0.85\nu \sim 0.86$ in this model.

V. QUANTUM FLUCTUATIONS

The Mott-insulator–superfluid-phase transition is driven by quantum fluctuations, which is common for quantum phase transitions. Here we show that a close connection also exists between quantum fluctuations and the phase transition of entanglement. In the dynamical regime of entanglement production, the system is required to undergo a delocalization process, where large quantum fluctuation exists, to generate entanglement. So the quantum phase transition of entanglement should be closely related to quantum fluctuations. In the angular momentum representation $|j,j_z\rangle$, where $j = N/2$ and $j_z = -N/2, -N/2+1, \ldots, N/2$, the quantum fluctuation is $(\Delta J_z)^2 = \langle J_z^2\rangle - \langle J_z\rangle^2$. We show that $(\Delta J_z)^2$ and $E(\rho)$ have a similar behavior, which indicates their close connection with each other. We plot $(\Delta J_z)^2$, $E(\rho)$ and their derivatives with respect to Ω in their reduced value in Fig. 4. We see that both the quantum fluctuation and the quantum entanglement grow with the external field Ω, and their growth corresponds to each other, which can be seen from their derivatives. As quantum entanglement is a nonclassical correlation, it is consistent that its quantum phase transition is closely related to quantum fluctuations.

There is a "delay" between the derivative of $E(\rho)$ and that of $(\Delta J_z)^2$, where the derivative of $E(\rho)$ reaches its maximum value earlier than the derivative of $(\Delta J_z)^2$. This is due to the finite-size effects. We are not working in the thermodynamic limit, so the derivatives between the quantum fluctuation and the quantum entanglement are not in complete correspondence. This is further confirmed by Table I, where the delay $\Delta\Omega$ between the maximum points of the derivatives is calculated for various system sizes. We see that the delay between them is decreasing as the system size grows, so we can figure that in the thermodynamic limit, the growth behavior of the entanglement and the fluctuation will approximately correspond to each other.

VI. SUMMARY

In summary, we have studied the entanglement of a boson system from the quantum-phase-transition approach. It is shown that in this system, there is a continuous phase transition

TABLE I. The "delay" $\Delta\Omega$ between the maximum points of the derivatives of $E(\rho)$ and $(\Delta J_z)^2$ for various system sizes. As the system size increases, the delay decreases, which means the growth behavior of the entanglement and the fluctuation are more closely related. This suggests that in the thermodynamic limit, the two growth behaviors will correspond to each other.

N	200	400	600	800	1600	2700
$\Delta\Omega$	0.000 675	0.000 375	0.000 263	0.000 188	0.000 075	0.000 055

for the nonlocal order parameter, and entanglement exhibits scaling behavior near the critical point, with the critical exponents calculated to be $\nu = 1.01$ and $\gamma = 0.86$. The critical behavior under discussion is different from that of the spin-lattice models because a power-law divergence is obtained for the boson system, while it is logarithmic divergence for the spin models. A further study of this phenomenon may consist of deriving an entanglement measure for boson systems of more lattice sites, i.e., investigating the quantum phase transition of the Bose-Hubbard model of more lattice sites and obtaining its universality class. The renormalization group method that is specifically used for taking into account the effect of quantum entanglement [26–28] may be used in that case.

ACKNOWLEDGMENTS

This project is partly supported by the National Natural Science Foundation of China (Grant No. 11105086), the National Research Foundation and Ministry of Education, Singapore (Grant No. WBS: R-710-000-008-271), the Natural Science Foundation of Shandong Province (Grant No. ZR2009AM026, BS2011DX029), the basic scientific research project of Qingdao (Grant No. 11-2-4-4-(6)-jch), the basic scientific research business expenses of the central university, and the Open Project of Key Laboratory for Magnetism and Magnetic Materials of the Ministry of Education, Lanzhou University.

[1] R. Horodecki, P. Horodecki, M. Horodecki, and K. Horodecki, Rev. Mod. Phys. **81**, 865 (2009).
[2] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. **80**, 517 (2008).
[3] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **54**, 3824 (1996).
[4] W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).
[5] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).
[6] T. Barthel, S. Dusuel, and J. Vidal, Phys. Rev. Lett. **97**, 220402 (2006).
[7] S.-J. Gu, S.-S. Deng, Y.-Q. Li, and H.-Q. Lin, Phys. Rev. Lett. **93**, 086402 (2004).
[8] D. Larsson and H. Johannesson, Phys. Rev. Lett. **95**, 196406 (2005).
[9] J. Vidal, R. Mosseri, and J. Dukelsky, Phys. Rev. A **69**, 054101 (2004).
[10] A. P. Hines, R. H. McKenzie, and G. J. Milburn, Phys. Rev. A **67**, 013609 (2003).
[11] A. J. Leggett, Rev. Mod. Phys. **73**, 307 (2001).
[12] H. T. Ng and P. T. Leung, Phys. Rev. A **71**, 013601 (2005).
[13] A. Sorensen, L. Duan, J. Cirac, and P. Zoller, Nature (London) **409**, 63 (2001).
[14] Y. Li, P. Treutlein, J. Reichel, and A. Sinatra, Eur. Phys. J. B **68**, 365 (2009).
[15] A. Tonel, J. Links, and A. Foerster, J. Phys. A **38**, 1235 (2005).
[16] J. Neumann, *Mathematische Grundlagen Der Quantenmechanik* (Springer, Berlin, 1995).
[17] M. P. A. Fisher, P. B. Weichman, G. Grinstein, and D. S. Fisher, Phys. Rev. B **40**, 546 (1989).
[18] I. Bloch, J. Dalibard, and W. Zwerger, Rev. Mod. Phys. **80**, 885 (2008).
[19] T. D. Kühner and H. Monien, Phys. Rev. B **58**, R14741 (1998).
[20] M. Greiner, O. Mandel, T. Esslinger, T. W. Hnsch, and I. Bloch, Nature (London) **415**, 39 (2002).
[21] N. Elstner and H. Monien, Phys. Rev. B **59**, 12184 (1999).
[22] L. Amico and V. Penna, Phys. Rev. Lett. **80**, 2189 (1998).
[23] R. Schützhold, M. Uhlmann, Y. Xu, and U. R. Fischer, Phys. Rev. Lett. **97**, 200601 (2006).
[24] J. D. Hunter, Comput. Sci. Eng. **9**, 90 (2007).
[25] E. Jones *et al.*, SciPy: Open source scientific tools for PYTHON (unpublished).
[26] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[27] T. J. Osborne and M. A. Nielsen, Quant. Inf. Proc. **1**, 45 (2002).
[28] T.-C. Wei, Phys. Rev. A **81**, 062313 (2010).