Scaling of entanglement at a quantum phase transition for a two-dimensional array of quantum dots

Jiaxiang Wang and Sabre Kais
Chemistry Department, Purdue University, West Lafayette, Indiana 47907, USA
(Received 19 November 2003; published 4 August 2004)

Using the Hubbard model, the entanglement scaling behavior in a two-dimensional itinerant system is investigated. It has been found that, on the two sides of the critical point denoting an inherent quantum phase transition (QPT), the entanglement follows different scalings with the size, just as an order parameter does. This fact reveals the subtle role played by the entanglement in QPT as a fungible physical resource.

DOI: 10.1103/PhysRevA.70.022301 PACS number(s): 03.67.Mn, 71.30.+h

The existence of entanglement between distinctive quantum systems has marked a fundamental difference between quantum and classical physics. Recently, with the explosive development of research in quantum information theory and quantum computation [1–4], the study of entanglement [5,6] has come into the limelight again after more than 60 years of controversies and strenuous progress. Experimentally, entanglements have already been produced between up to four photons [7,8] and even between two macroscopic states such as two superconducting qubits, each of which contains as many as 10^9 electrons [9]. But theoretically, because an ensemble's Hilbert space grows exponentially with the number of its component particles, we are still far from fully understanding the contents of the entanglements. Only for the simplest state with two distinguishable particles can we have a complete description of the entanglement measure. For states of more than two particles, especially for mixed states, the current knowledge about their entanglement is very limited, and all the related complexities have just begun to be explored. For the spin-only entanglement of localized distinguishable particles, the most popular measure of the entanglement is the Wootters measure [10]. Recently, the influence of quantum statistics on the definition of entanglement has begun to be noticed and discussed by several authors [11–13]. Although various entanglement measures have been put forward, according to Gitting's criterions [15], only Zanardi's measure [16] survives the test of all the requirements upon entanglement definition. This measure is given in Fock space as the von Neuman entropy, namely,

$$E_j = -\operatorname{Tr} \rho_j \ln \rho_j, \quad \rho_j = \operatorname{Tr}_j |\psi\rangle\langle\psi|, \tag{1}$$

where Tr_j denotes the trace over all but the jth site and ψ is the antisymmetric wave function of the studied system. Hence, E_j actually describes the entanglement of the jth site with the remaining sites. A generalization of this one-site entanglement is to define an entanglement between one L-site block with the rest of the systems [17],

$$E_L = -\operatorname{Tr}(\rho_L \log_2 \rho_L), \tag{2}$$

where all the sites are traced out except those belonging to the selected block.

Recently, it has been speculated that the most entangled systems could be found at the critical point when the system undergoes a quantum phase transition (QPT), i. e., a qualitative change of some physical properties takes place as an order parameter in the Hamiltonian is tuned [18]. QPT results from quantum fluctuations at the absolute zero of temperature and is a pure quantum effect featured by long-range correlations. So far, there have already been some efforts in exploring the above speculations, such as the analysis of the *XY* model about the single-spin entropies and two-spin quantum correlations [19,20], the entanglement between a block of L contiguous sites and the rest of the chain [17], and also the scaling of entanglement near QPT [21]. But because there is still no analytical proof, the role played by the entanglement in quantum critical phenomena remains elusive. Generally speaking, there exist at least two difficulties in resolving this issue. First, only two-particle entanglement has been well explored. How to quantify the multiparticle entanglement is not clear. Second, QPT closely relates to the notorious many-body problems, which is almost analytically intractable. The only effective and accurate way to deal with QPT in a critical region was the density-matrix renormalization group method [22]. Unfortunately, it is only efficient for one-dimensional cases because of the much more complicated boundary conditions for two-dimensional situation. It should be mentioned here that recently, Vial [23] has put forward another new efficient numerical method to study one-dimensional many-body systems based upon the entanglement contained in the system.

In this paper, we will focus on investigating the entanglement behavior in QPT for a two-dimensional array of quantum dots, which provides a suitable arena for the implementation of quantum computation [24–26]. For this purpose, the real-space renormalization group technique [27] will be utilized and developed for the finite-size analysis of entanglement.

The model we use is the Hubbard model with the Hamiltonian,

$$H = -t \sum_{\langle i,j\rangle,\sigma} [c_{i\sigma}^{\dagger} c_{j\sigma} + \text{H . c.}] + U \sum_i \left(\frac{1}{2} - n_{i\uparrow}\right)\left(\frac{1}{2} - n_{i\downarrow}\right) + K \sum_i I_i, \tag{3}$$

where t is the nearest-neighbor hopping term, U is the local

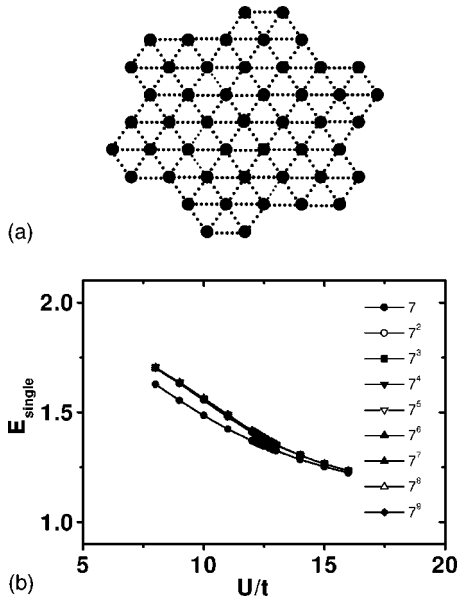

FIG. 1. (a) A schematic diagram showing the central site and the surrounding ones in the triangular quantum dot lattice. The dotted lines represent the site-site interactions. (b) Scaling of the single-site entanglement for various system sizes. The sizes are denoted by different symbols.

repulsive interaction, $K=-U/4$, and I_i is the unit operator. $c_{i\sigma}^{\dagger}(c_{i\sigma})$ creates (annihilates) an electron with spin σ in a Wannier orbital located at site i; the corresponding number operator is $n_{i\sigma}=c_{i\sigma}^{\dagger}c_{i\sigma}$ and $\langle\rangle$ denotes the nearest-neighbor pairs. H.c. denotes the Hermitian conjugate.

For a half-filled triangular quantum lattice, there exists a metal-insulator phase transition with the tuning parameter U/t at the critical point 12.5 [28–30]. The corresponding order parameter for metal-insulator transition is the charge gap defined by $\Delta_g=E(N_e-1)+E(N_e+1)-2E(N_e)$, where $E(N_e)$ denotes the lowest energy for a N_e electron system. In our case, N_e is equal to the site number N_s of the lattice. Unlike the charge gap calculated from the energy levels, the Zanardi's measure of the entanglement is defined upon the wave function corresponding to $E(N_e)$ instead. Using the conventional renormalization group method for the finite-size scaling analysis [28–30], we can discuss three schemes of entanglement scaling: (1) Single-site entanglement scaling with the total system size, E_{single}, (2) block-block entanglement scaling with the block size, E_{block}, and (3) single-block entanglement scaling with the block size, $E_{block-block}$.

Figure 1 presents the single-site entanglement scaling. It is obvious that E_{single} is not a universal quantity. This conclusion is consistent with the argument given by Osborne [19], who claims that the single-site entanglement is not scalable because it does not own the proper extensivity and does not distinguish the local and distributed entanglement. One more interesting feature in Fig. 1 is that when the system size is increased beyond 7^2, E_{single} makes almost no change any more. This implies that only a limited region of sites around the central site contributed significantly to the single-site entanglement.

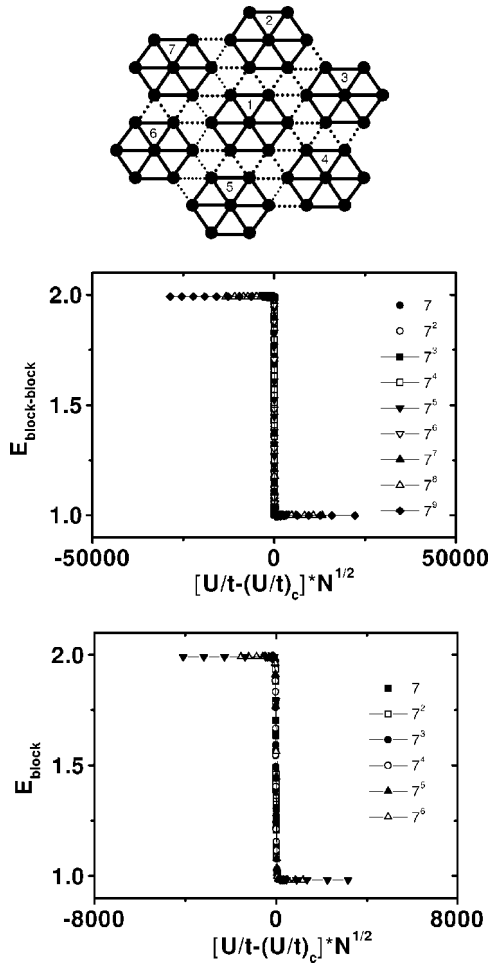

FIG. 2. (a) The schematic diagram displays the lattice configuration with a central block and the surrounding ones. (b) Scaling of block-block for various system sizes and (c) scaling of block entanglements with the block size.

Using the one-parameter scaling theory, near the phase-transition point, we assume the existence of scaling function f for $E_{block-block}$ such that

$$E_{block-block}=q^{y_E}f\left(\frac{L}{\xi}\right), \tag{4}$$

where $q=U/t-(U/t)_c$ measures the deviation distance of the system away from the critical state with $(U/t)_c=12.5$, which is exactly equal to the critical value for metal-insulator transition when the same order parameter U/t is used [28–30]. $\xi=q^{-\nu}$ is the correlation length of the system with the critical exponent ν.

Hence,

$$E_{block-block}=q^{y_E}f(N^{1/2\upsilon}q), \tag{5}$$

where we used $N=L^2$ for the two-dimensional systems.

In Fig. 2, we show the results of $E_{block-block}$ as a function of (U/t) for different system sizes. With proper scaling, all the curves collapse onto one curve, which can be expressed as

$$E_{block-block} = f(qN^{1/2}). \tag{6}$$

Thus, the critical exponents in Eq. (5) are $y_E=0, \nu=1$. It is interesting to note that we obtained the same ν as in the study of metal-insulator transition. This shows the consistency of the results, since the critical exponent ν is only dependent on the inherent symmetry and dimension of the investigated system.

Another significant result lies in the finding that the metal state is highly entangled, while the insulating state, is only partly entangled. For a four-dimensional density matrix, the maximally entangled state can be written as a diagonal matrix with equal components $\frac{1}{4}$. The related entanglement is $-\Sigma_{i=1}^{4}\frac{1}{4}\log_2\frac{1}{4}=2$, which is exactly the value obtained from Fig. 2(b). However, unlike the metal state, the insulating states should be expected to have electrons showing less mobility. If we assume the highly probable situation, i.e., that the central site has equal probability to be in $|\uparrow\rangle$, $|\downarrow\rangle$ and no occupation in $|0\rangle$, $|\uparrow\downarrow\rangle$, the corresponding entanglement is then $E_{block-block}=-\Sigma_{i=2}^{3}\frac{1}{2}\log_2\frac{1}{2}=1$, also consistent with the results from Fig. 2(b).

All the above discussions are confined to the entanglement between the central block and its surrounding blocks. Because the central block is a very special one showing the highest symmetry, one may wonder what can happen to the neighboring blocks, for example, the entanglement between block 7 and the rest of the six blocks. To answer this question, the same calculations are conducted and the results are the same except that in the metal state, the maximal entanglement is a little less than 2 and the minimal one is a little less than 1. This can be explained by the asymmetric position of site 1 in the block.

It should be mentioned that the calculated entanglement here has a corresponding critical exponent $y_E=0$. This means that the entanglement is constant at the critical point over all sizes of the system. But it is not a constant over all values of U/t. There is an abrupt jump across the critical point as $L \rightarrow \infty$.

If we divide the regime of the order parameter into the noncritical regime and the critical regime, the results can be summarized as follows: In the noncritical regime, i.e., U/t is away from $(U/t)_c$, as L increases, the entanglement will saturate onto two different values depending on the sign of $U/t - (U/t)_c$. At the critical point, the entanglement is actually a constant independent of size L.

These properties are qualitatively different from the single-site entanglement discussed by Osborne [19], where the entanglement with Zanardi's measure increases from zero to the maximum at the critical point and then decreases again to zero as the order parameter γ for the XY mode is tuned.

These peculiar properties of the entanglement we have found here can be of potential interest to make an effective ideal "entanglement switch." For example, with seven blocks of quantum dots on a triangular lattice, the entanglement among the blocks can be regulated as "0" or "1" almost immediately once the tuning parameter U/t crosses the critical point. The switch errors will depend on the size of the blocks. Since it has already been a well-developed technique to change U/t for the quantum dot lattice [26,31], the above scheme should be workable. To remove the special confinement we have made upon the calculated entanglement, namely only the entanglement of block 1 and block 7 with the rest of the blocks are considered. In the following, we will prove that the average pairwise entanglement also has the properties shown in Fig. 2(b).

Let $E_{block-block,7}$ denote the entanglement between the 7th and all the remaining blocks in a hexagonal system. From the symmetry of the system we can show that the total pairwise entanglement $E_{tot}=6E_{block-block}+3E_{block-block,7}$. The average two-site entanglement is $E_{average}=E_{tot}/21=(2E_{block-block}+E_{block-block,7})/7$. Because

$$E_{block,7} = g_1(qN^{1/2}), \quad E_{block,1} = g_2(qN^{1/2}), \tag{7}$$

then we should have $E_{average}=g(qN^{1/2})$, where g_1, g_2, and g are scaling functions.

For obtaining the single-block entanglement, the first step is to make a cutoff over the system size. In our work, we let it be 7^9. The results are presented in Fig. 2(c). It is magnificent that as we change the size of the central block, its entanglement with all the rest of the sites follows the same scaling properties as $E_{block-block}$. It is understandable if we consider the fact that only a limited region around the block contributes mostly to E_{block}. This result greatly facilitates the fabrication of realistic entanglement control devices, such as quantum gates for a quantum computer, since we don't need to delicately care about the number of component blocks in fear that the next neighboring or the next-next neighboring quantum dots should influence the switching effect.

In summary, in this paper, various schemes of the finite-size scaling properties with Zanardi's measure of entanglement, the von Neuman entropy Eq. (1), has been investigated for the Hubbard model on a triangular quantum lattice. The critical exponent $\nu=1$ has been found, which coincides well with our previous work in studying a quite different physical property, the charge gap. When the block size $L \rightarrow \infty$, the entanglement shows an abrupt change when the tuning parameter crosses the phase-transition point. This property might be applied to make an "entanglement switch," and shows the promising prospect of regarding entanglement as a physical resource.

We would like to acknowledge the financial support of the National Science Foundation

[1] K. Mattle, H. Weinfurter, P. G. Kwiat, and A. Zeilinger, Phys. Rev. Lett. **76**, 4656 (1996).
[2] D. Bouwmeester, J. Pan, K. Mattle, M. Eibl, H. Weinfurter, and A. Zeilinger, Nature (London) **390**, 575 (1997).
[3] T. Jennewein, C. Simon, G. Weihs, H. Weinfurter, and A. Zeilinger, Phys. Rev. Lett. **84**, 4729 (2000).
[4] L. M. K. Vandersypen, M. Steffen, G. Breyta, C. S. Yannoni, M. H. Sherwood, and I. L. Chuang, Nature (London) **414**, 883 (2001).
[5] M. Lewenstein, D. Bruss, J. I. Cirac, B. Kraus, M. Ku, J. Samsonowicz, A. Sanpera, and R. Tarrach, J. Mod. Opt. **47**, 2841 (2000).
[6] D. Bruss, J. Math. Phys. **43**, 4237 (2002).
[7] A. Lamas-Linares, J. C. Howell, and D. Bouwmeester, Nature (London) **412**, 887 (2001).
[8] M. Eibl, S. Gaertner, M. Bourennane, C. Kurtsiefer, M. Zukowski, and H. Weinfurter, Phys. Rev. Lett. **90**, 200403 (2003).
[9] A. J. Berkley, H. Xu, R. C. Ramos, M. A. Gubrud, F. W. Strauch, P. R. Johnson, J. R. Anderson, A. J. Dragt, C. J. Lobb, and F. C. Wellstood, Nature (London) **300**, 1548 (2003).
[10] W. K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).
[11] J. Schliemann, J. Ignacio Cirac, M. Kus, M. Lewenstein, and D. Loss, Phys. Rev. A **64**, 022303 (2001).
[12] Y. S. Li, B. Zeng, X. S. Liu, and G. L. Long, Phys. Rev. A **64**, 054302 (2001).
[13] D. Aharonov, Phys. Rev. A **62**, 062311 (2000).
[14] P. Zanardi and X. Wang, J. Phys. A **35**, 7947 (2002).
[15] J. R. Gittings and A. J. Fisher, Phys. Rev. A **66**, 032305 (2002).
[16] P. Zanardi, Phys. Rev. A **65**, 042101 (2002).
[17] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, e-print quant-ph/0211074.
[18] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 1999).
[19] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002); e-print quant-ph/0109024.
[20] O. Osenda, Z. Huang, and S. Kais, Phys. Rev. A **67**, 062321 (2003).
[21] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).
[22] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[23] G. Vidal, e-print quant-ph/0301063; e-print quant-ph/0310089; J. I. Latorre, E. Rico, G. Vidal, e-print quant-ph/0304098.
[24] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).
[25] G. Burkard, D. Loss, and D. P. DiVincenzo, Phys. Rev. B **59**, 2070 (1999).
[26] X. Hu and S. Das Sarma, Phys. Rev. A **61**, 062301 (2000).
[27] *Real-Space Renormalization*, edited by T. W. Burkhardt and J. M. J. van Leeuwen, Topics in Current Physics (Springer, New York, 1982).
[28] J. X. Wang, S. Kais, and R. D. Levine, Int. J. Mol. Sci. **3**, 4 (2002).
[29] J. X. Wang and S. Kais, Phys. Rev. B **66**, 081101(R) (2002).
[30] J. X. Wang, S. Kais, F. Remacle, and R. D. Levine, J. Phys. Chem. B **106**, 12847 (2002).
[31] F. Remacle and R. D. Levine, ChemPhysChem **2**, 20 (2001).