Entanglement and Quantum Phase Transition in a One-Dimensional System of quantum Dots with Disorder

Hefeng Wang and Sabre Kais *

Department of Chemistry, Purdue University, West Lafayette, IN 47907

Abstract

We study the entanglement of formation and quantum phase transition in a one-dimensional quantum dots system with disorder modeled by the Hubbard Hamiltonian. The entanglement for three different cases has been studied: The pure case; the impurity case of a symmetric electron hopping and an impurity case of an asymmetric electron hopping. We have found that the local entanglement of the system can be tuned by introducing different impurities characterized by the physical parameters of the system. In particular, for certain parameters, the entanglement is negligible up to a critical point U_c, where a quantum phase transition occurs, and is different from zero above U_c.

* Corresponding author: kais@purdue.edu

I. INTRODUCTION

After the work of Benioff[1], Feynman[2] and Deutsch[3] in the field of quantum computing and quantum information, the development in this area has been explosive[4, 5]. The intrinsic parallelism in quantum mechanics due to superposition has been shown to lead to greater computational power for a quantum computer. When quantum error correction is shown to be possible[8], people started looking for physical systems that are appropriate for a qubit, thus to build a quantum computer. Among many suggestions, quantum computer based on quantum dots is a prominent one[9, 10]. Quantum dots are clusters of atoms and molecules that are small enough so that their electronic states are discrete. To describe the quantum dots, a simple approximation is to regard each dot as having a valence orbital, the electron occupation could be $|0>$, $|\uparrow>$, $|\downarrow>$ and $|\uparrow\downarrow>$, with other electrons treated as core electrons[11]. The valence electron can tunnel from a given dot to its nearest neighbor obeying the Pauli principle and thereby two dots can be coupled. This is the electron hopping effect, which can be characterized by the distance between two dots. Another effect that needs to be considered is the electron repulsion on each dot, which can be characterized by the size of the dots. These two effects can be described by the electron hopping parameter t and the Coulomb repulsion parameter U, by adjusting these two parameters, one can tune the entanglement of the system, which is very important in quantum information processing.

Quantum entanglement is one of the most important concepts in quantum information theory and quantum computation[12–15]. The non-local correlations exhibited by the states of quantum systems are key to the implementation of quantum information processing technologies [16–23]. It has been realized that quantum entanglement can be used as a controllable physical resource[24]. Quantum entanglement is also relevant to quantum phase transition. Osterloh et.al[25] among others[26–28] connected the theory of critical phenomena with quantum information by exploring the entangling resources of a system close to the quantum critical point in a class of one-dimensional magnetic systems. Recently[29], we have demonstrated that for a class of one-dimensional magnetic systems entanglement can be controlled and tuned by varying the anisotropic parameter in the XY-Hamiltonian and by introducing impurities into the systems in the equilibrium state. Gu *et al.*[35] show that for the one-dimensional extended Hubbard model, quantum phase transition can be identified at places where local entanglement is maximum or its derivative is singular.

Finding a measure of the quantum entanglement is an important issue in the field of quantum information and computation. For a fermion system, there exist several measures of the quantum entanglement, the Wootters' measure for the spin-only entanglement of localized distinguishable particles[30], the Schliemann's measure[31, 32] and Zanardi's measure[33]. In this paper, we will follow the work of Gittings and Fisher[34] by using the von Neumann entropy as an entanglement measure, to study the entanglement of formation in the one-dimensional Hubbard model when disorder of electron hopping is introduced.

II. ENTANGLEMENT IN THE ONE-DIMENSIONAL HUBBARD MODEL

We consider an array of quantum dots modeled by the one-dimensional Hubbard Hamiltonian of the form

$$H = -\sum_{<ij>,\sigma} t_{ij}\ c^{+}_{i\sigma}\ c_{j\sigma} + U\sum_{i}\ n_{i\uparrow}\ n_{i\downarrow} \tag{1}$$

where t_{ij} stands for the hopping between the nearest neighbor sites for the electrons with the same spin, i and j are the neighboring site numbers, σ is the electron spin, $c^{+}_{i\sigma}$ and $c_{j\sigma}$ are the creation and annihilation operators, U is the Coulomb repulsion for the electrons on the same site. The periodic boundary condition is applied.

The entanglement measure is given by von Neumann entropy[33]

$$E_j = -Tr(\rho_j log_2 \rho_j), \qquad \rho_j = Tr_j(|\Psi><\Psi|) \tag{2}$$

where Tr_j denotes the trace over all but the jth site, $|\Psi>$ is the antisymmetric wavefunction of the fermions system and ρ_j is the reduced density matrix. Hence E_j actually describes the entanglement of the jth site with the remaining sites.

In the Hubbard model, the electron occupation of each site has four possibilities, there are four possible local states at each site, $|\nu>_j = |0>_j, |\uparrow>_j, |\downarrow>_j, |\uparrow\downarrow>_j$. The dimensions of the Hilbert space of an L-site system is 4^L and $|\nu_1\nu_2...\nu_L>=\prod_{j=1}^{L}|\nu_j>_j$ can be used as basis vectors for the system. The entanglement of the jth site with the other sites is given by[35]

$$E_j = -zLog_2 z - u^{+}Log_2 u^{+} - u^{-}Log_2 u^{-} - wLog_2 w, \tag{3}$$

where the local density matrix is site independent since the Hamiltonian is invariant under translation and is given by

$$\rho_j = z|0><0| + u^+|\uparrow><\uparrow| + u^-|\downarrow><\downarrow| + w|\uparrow\downarrow><\uparrow\downarrow| \tag{4}$$

with

$$w =< n_{j\uparrow} n_{j\downarrow} >= Tr(n_{j\uparrow} n_{j\downarrow} \rho_j) \tag{5}$$

$$u^+ =< n_{j\uparrow} > -w, \qquad u^- =< n_{j\downarrow} > -w \tag{6}$$

$$z = 1 - u^+ - u^- - w = 1 - < n_{j\uparrow} > - < n_{j\downarrow} > + w. \tag{7}$$

The Hubbard Hamiltonian can be rescaled by dividing it with the electron hopping parameter $t = t_{ij}$. Thus, after rescaling the electron repulsion becomes U/t.

In the ideal case, we can expect an array of the quantum dots to have the same size and distributed evenly, so that the parameters t and U are the same everywhere respectively. We call this the pure case. In fact the size of the dots may not be the same and they may not be evenly distributed, which we call the impurity case. In this paper, we consider two types of impurities. The first one is to introduce a symmetric hopping impurity t' between two neighboring dots and the rest of the sites with hopping parameter t, the second one is to introduce an asymmetric electron hopping t' between two neighboring dots, the right hopping is different from the left hopping, while the rest of the sites with hopping parameter t.

A. Pure Case

In the pure case, for the one-dimensional Hubbard model with half-filling electrons, we have $< n_\uparrow >=< n_\downarrow >= \frac{1}{2}$, $u^+ = u^- = \frac{1}{2} - w$, and the entanglement is given by

$$E_j = -2w log_2 w - 2(\frac{1}{2} - w) log_2(\frac{1}{2} - w) \tag{8}$$

Consider the particle-hole symmetry of the one-dimensional Hubbard model, one can obtain $w(-U) = \frac{1}{2} - w(U)$, so the entanglement is an even function of U, $E_j(-U) = E_j(U)$. The minimum of the entanglement is 1 as $U \to \pm\infty$. As $U \to +\infty$ all the sites are singly occupied the only difference is the spin of the electrons on each site, which can be referred as spin entanglement. As $U \to -\infty$, all the sites are either doubly occupied or empty, which

is referred as space entanglement. The maximum of the entanglement is 2 at U=0, which is the sum of the spin and space entanglement of the system. The ground state of the one-dimensional Hubbard model at half filling is metallic for $U < 0$, and insulating for $U > 0$, $U = 0$ is the critical point for the metal insulator transition, where the local entanglement reaches its maximum. In figure (1) we show the entanglement as a function U/t for six sites and six electrons. Our results are in complete agreement with exact one obtained by Bethe ansatz[35].

The good agreement for the calculated entanglement obtained from the Bethe ansatz (number of sites equals 70 and ∞) and exact diagonalization technique (number of sites equals 10)[35] and our calculations (number of sites equals 6) justifies the validity of our results using small clusters of sites to study other impurity cases.

B. Impurity Case A: Symmetric Electron Hopping

In this case we introduce an impurity of symmetric electron hopping in the first two sites, $t' = t_{21} = t_{12} = t(1 + \alpha)$, the electron hopping on the rest of the sites is still scaled as t. Figure (2) shows the entanglement of sites 1 and 2, as a function of U/t, with $\alpha = 0, 1, 2, 3$. From figure (2), we can see that the minimum entanglement is 1 as $U \to \pm\infty$, and the maximum entanglement is 2 at $U = 0$. The local entanglement on sites 1 and 2 as well as on other sites are symmetric. The only difference from the pure case is that the curve becomes broader, since as α increases the quantity $|U/t'|$ decreases. Physically, this means that the contribution from space entanglement (as $U/t > 0$) or spin entanglement (as $U/t < 0$) increases as $|U/t|$ close to 0. The features displayed by the entanglement indicates that for the ground state of the one-dimensional Hubbard model at half filling when an impurity of symmetric electron hopping is introduced, the critical point $U_c = 0$ separate the metal phase from the insulator phase. Thus, at this critical point the system undergoes a quantum phase transition.

C. Impurity Case B: Asymmetric Electron Hopping

An impurity of asymmetric electron hopping can also be introduced to the pure case, which could happen when the dots are in different potentials. We set the electron hopping

from site 1 to site 2 as $t' = t_{21} = t(1+\alpha)$. However, the hoping from site 2 to site 1 as well as all other electron hopping are t. We can obtain the entanglement on sites 1 and 2 with $\alpha = 0, 1, 2, 3$ as shown in figure(3). The entanglement is no longer symmetric when the asymmetric impurity is introduced, the maximum of the entanglement shifts from $U = 0$, and is less than 2. The minimum of the entanglement is less than 1 and decreases as α increases when $U \to -\infty$. The entanglement goes to 1 as $U \to +\infty$. This can be explained as in the half filling model, when $U \to +\infty$ all the sites are singly occupied and the occupation number of spin-up electrons equals the occupation number of spin-down electrons; when $U \to -\infty$, since the electron hopping from site 1 to site 2 is easier such that the occupation number $w =< n_{1\uparrow} n_{1\downarrow} >$ on site 1 is smaller and on site 2 is bigger, they compensate each other, the entanglement on these two sites are exactly the same. When $U/t < 0$, where the space entanglement makes up the main contribution to total entanglement of the system, the probability of site 1 and site 2 to be doubly occupied and empty is not balanced, this causes the entanglement to be lower than 1. This feature is more clear when α is increased, figure (4) shows how the entanglement when α is set to 1000. Here the interesting point is that the maximum entanglement can be reached at $U > 0$, which means that the state corresponding to the maximum entanglement can be obtained by adjusting the parameters t, t' and U. The same feature can also be obtained from the entanglement on the other sites. Figure (5) shows the local entanglement of sites 3 and 6 and the local entanglement of sites 4 and 5 when $\alpha = 1000$. The local entanglement for sites 3 and 6 are the same, also sites 4 and 5 are the same since each pair are in the same environment. They are symmetric with respect to the impurity introduced between sites 1 and 2 in the system. The entanglement on these two pairs of sites have the same feature as that of sites 1 and 2, this feature decreases as the sites are far away from the sites 1 and 2, where impurity is introduced. This feature of the local entanglement on each site of the system indicates that for the ground state of the one-dimensional Hubbard model at half filling when an asymmetric impurity of electron hopping is introduced, the critical point for the quantum phase transition occurs at a point $U_c > 0$. When $U \leq U_c$ the system is metallic and when $U > U_c$ the system is insulating. For the one-dimensional Hubbard model system, when an asymmetric electron hopping impurity is introduced, we can imagine that there is another site above the one-dimensional chain between sites 1 and 2 the electron can also hopping through this site, so an extra channel for electron hopping is introduced. In fact

such a system can be viewed as a two-dimensional system. In our previous study[36], we have shown the existence of the critical point at $U_c > 0$ for metal-insulator transition (MIT) and the close relation with the entanglement for two-dimensional Hubbard model systems.

In summary, we have studied the entanglement of an array of quantum dots modeled by the one-dimensional Hubbard Hamiltonian in three different cases. The entanglement in the pure case and the impurity of symmetric electron hopping case A is maximum at the critical point $U_c = 0$ for the metal insulator transition. In the asymmetric electron hopping case B the maximum of the entanglement indicates a critical point at $U_c > 0$. Moreover, we have found that the local entanglement of the system can be tuned by introducing different impurities characterized by the system parameters U, t and t'. In particular, for certain parameters, the entanglement is very small up to a critical point U_c, where a quantum phase transition occurs, and is different from zero above U_c. This can be used in quantum information processing where entanglement plays an important role. The system can be prepared to the desired state contains a certain amount of entanglement, then some quantum operation can be applied to the system for quantum control.

[1] P. Benioff, J. Stat. Phys. **563**, 22 (1980); Phys. Rev. Lett. **48**, 1581 (1982).

[2] R. P. Feynman, Int. J. Theor. Phys. **21**, 467 (1982).

[3] D. Deutsch, Proc. R. Soc. **A400**, 97 (1985); Proc. R. Soc. **A425**, 73 (1989).

[4] C. H. Bennett and D. P. DiVincenzo, Nature **404**, 247 (2000).

[5] C. Monroe, Nature **416**, 238 (2002).

[6] P. Shor, in *Proceedings of the 35th Annual Symposium on the Foundations of Computer Science*, ed. By S. Goldwasser (IEEE Computer Society, Los Alamitos, 1994), p. 124.

[7] L. K. Grover, Phys. Rev. Lett. **79**, 325 (1997).

[8] P. Shor, Phys. Rev. A **52**, R2493 (1995); A. Steane, Phys. Rev. Lett. **77**, 793 (1996).

[9] D. Loss, D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998)

[10] M. Friesen, M. P. Rugheimer, D. Savage, M. Lagally, D. van der Weide, R. Joynt, Phys. Rev. B **67**, 121301 (2003).

[11] F. Remacle and R. D. Levine, PNAS, **97**, 553 (2000)

[12] C.H. Bennett and D.P. DiVincenzo, Nature **404**, 247 (2000).

[13] C. Macchiavello, G.M. Palma and A. Zeilinger, *Quantum Computation and Quantum Information Theory* (World Scientific, 2000).

[14] M. Nielsen and I. Chuang *Quantum Computation and Quantum Communication* (Cambridge Univ. Press, Cambridge, 2000)

[15] J. Gruska, *Quantum Computing* (McGraw-Hill, 1999)

[16] V. Vedral, M.B. Plenio, M.A. Rippin and P.L. Knight, Phys. Rev. Lett. **78**, 2275 (1997).

[17] C.H. Bennett et. al. Phys. Rev. Lett. **70**, 1895 (1993).

[18] D. Bouwmeester et. al. Nature, **390**, 575 (1997).

[19] C.H. Bennett and S.J. Wiesener, Phys. Rev. Lett. **69**, 2881 (1992).

[20] A.K. Ekert, Phys. Rev. Lett.**67** , 661 (1991).

[21] M. Murao, D. Jonathan, M.B. Plenio and V. Vedral Phys. Rev. A **59**, 156 (1999).

[22] D. Bacon, J. Kempe, D.A. Lidar and K.B. Whaley, Phys. Rev. Lett. **85**, 1758 (2000).

[23] J. Vala, Z. Amitay, B. Zhang, S. R. Leone, and R. Kosloff, Phys. Rev. A **66**, 062316 (2002).

[24] M. A. Nielsen, C. M. Dawson, J. L. Dodd, A. Gilchrist, D. Mortimer, T. J. Osborne, M. J. Bremner, A. W. Harrow and A. Hines, Phys. Rev. A **67**, 052301 (2003).

[25] A. Osterloh, L. Amico, G. Falci, and Rosario Fazio, Nature **416**, 608 (2002).

[26] A. R, Its, B.Q. Jin and V.E. Korepin, J. Phys. A **38**, 2975 (2005).

[27] V.E. Korepin, Phys. Rev. Lett. **92**, 096402 (2004).

[28] F. Verstraete, M.A. Martin-Delgado, J.I. Cirac, Phys. Rev. Lett. **92**, 087201 (2004).

[29] O. Osenda, Z. Huang and S. Kais, Phys. Rev. A 67, 062321 (2003).

[30] W. K. Wooters, Phys. Rev. Lett. **80**, 2245 (1998).

[31] J. Schliemann, J. Ignacio Cirac, M. Kus, M. Lewenstein and D. Loss, Phys. Rev. A **64**, 022303 (2001).

[32] J. Schliemann, D. Loss and A. H. MacDonald, e-print, cond-mat/0009083.

[33] P. Zanardi, Phys. Rev. A **65**, 042101 (2002).

[34] J. R. Gittings and A. J. Fisher, Phys. Rev. A **66**, 032305 (2002).

[35] S. Gu, S. Deng, Y. Li, and H. Lin, Phys. Rev. Lett. **93**, 086402 (2004).

[36] J. Wang and S. Kais, Int. J. Quant. Chem. **93**, 360 (2003).

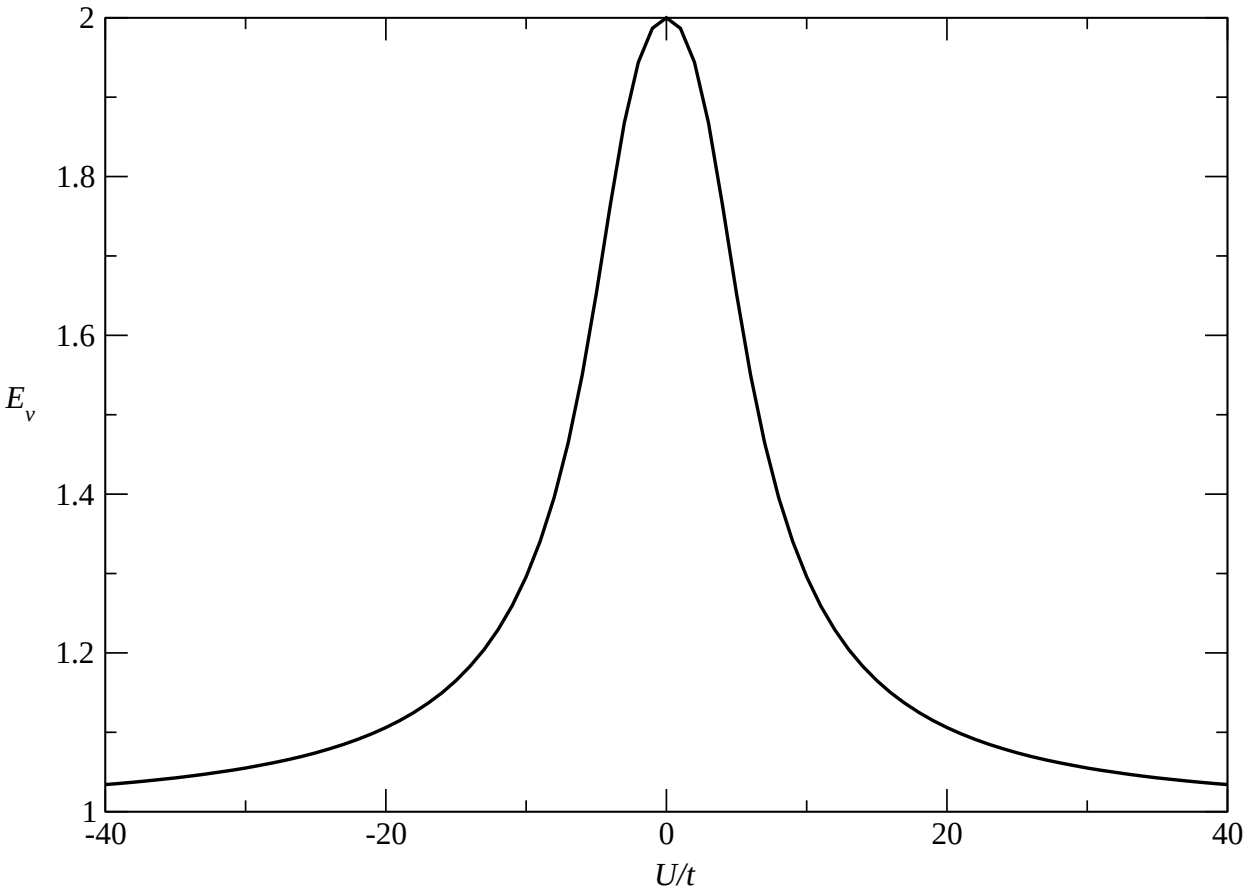

FIG. 1: Local entanglement given by von Neumann entropy, E_v, versus U/t in the pure case.

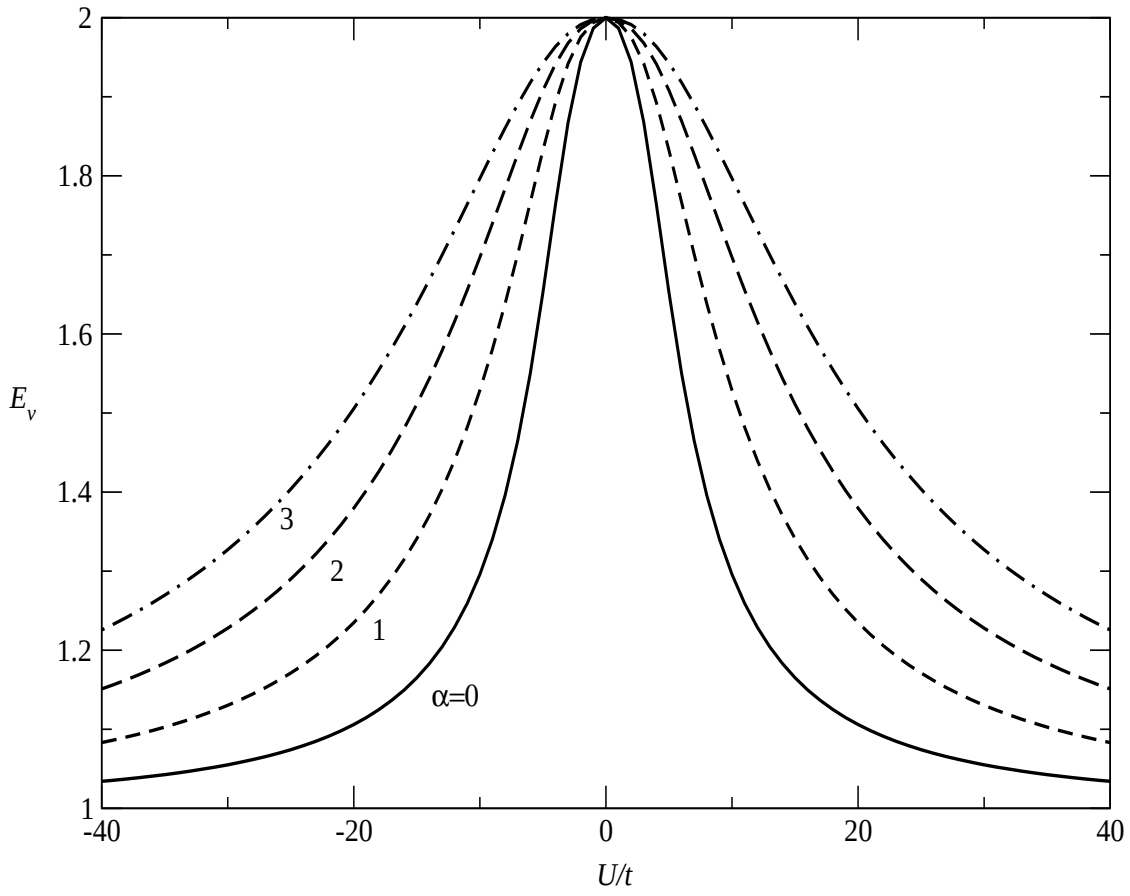

FIG. 2: Local entanglement E_v of sites 1 and 2 versus U/t in the symmetric electron hopping case.

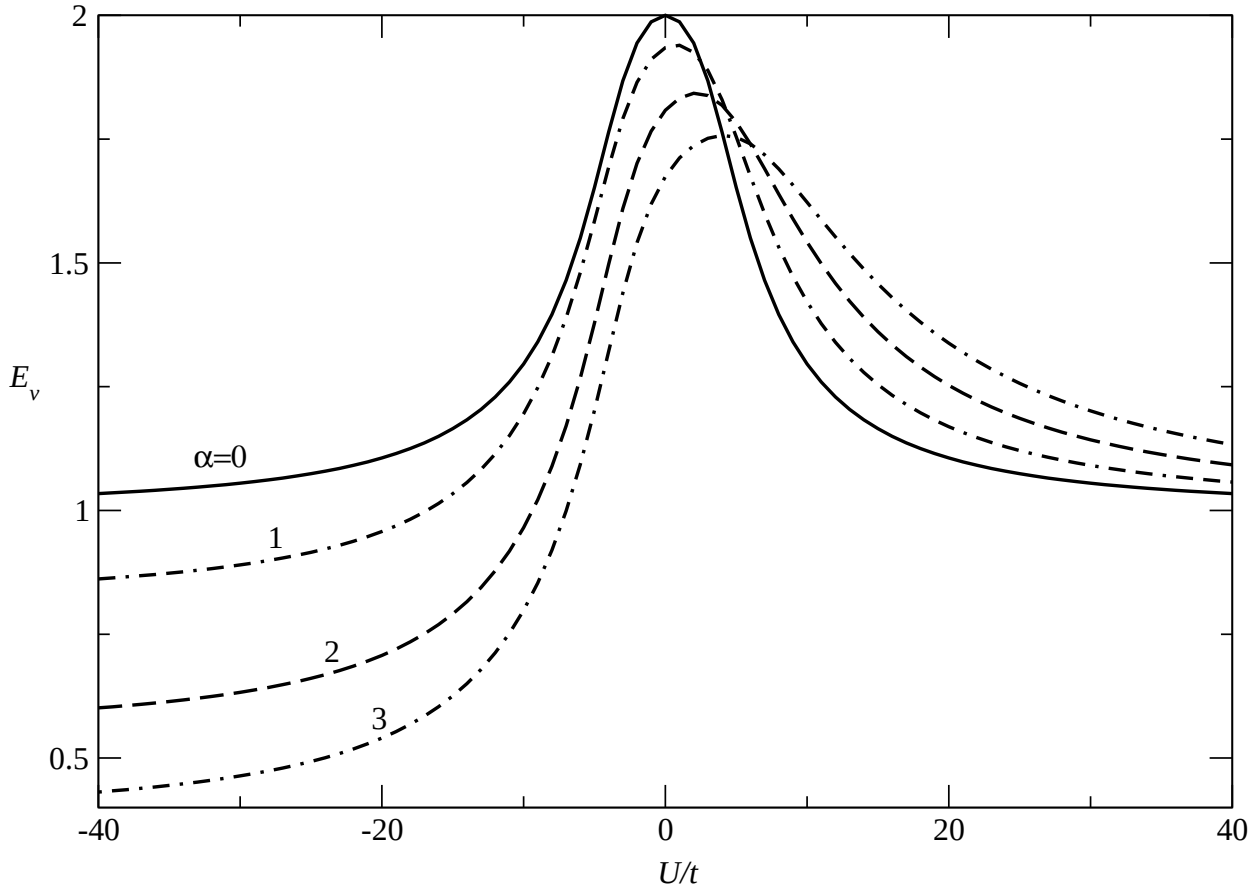

FIG. 3: Local entanglement E_v of sites 1 and 2 versus U/t in the asymmetric electron hopping case.

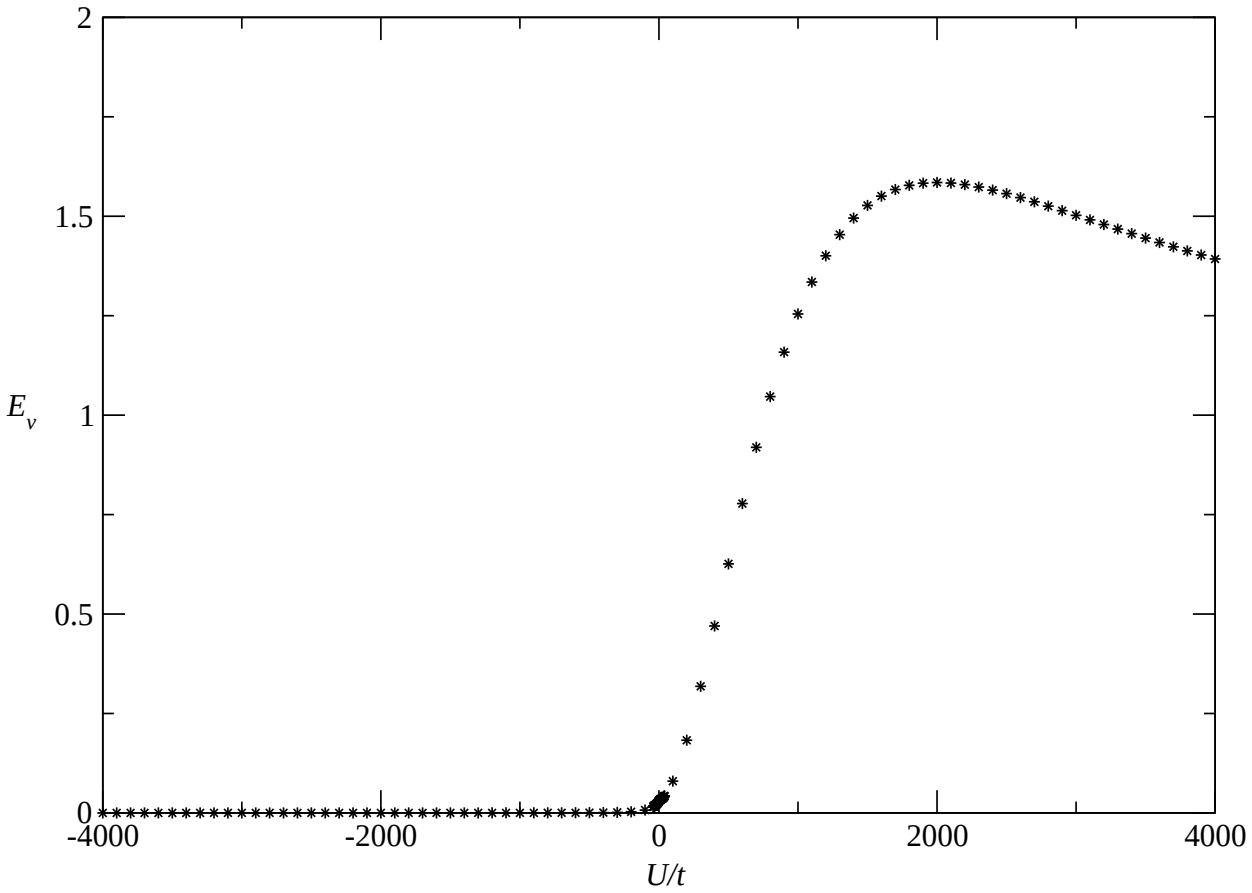

FIG. 4: Local entanglement E_v of sites 1 and 2 versus U/t in the asymmetric electron hopping case with $\alpha = 1000$

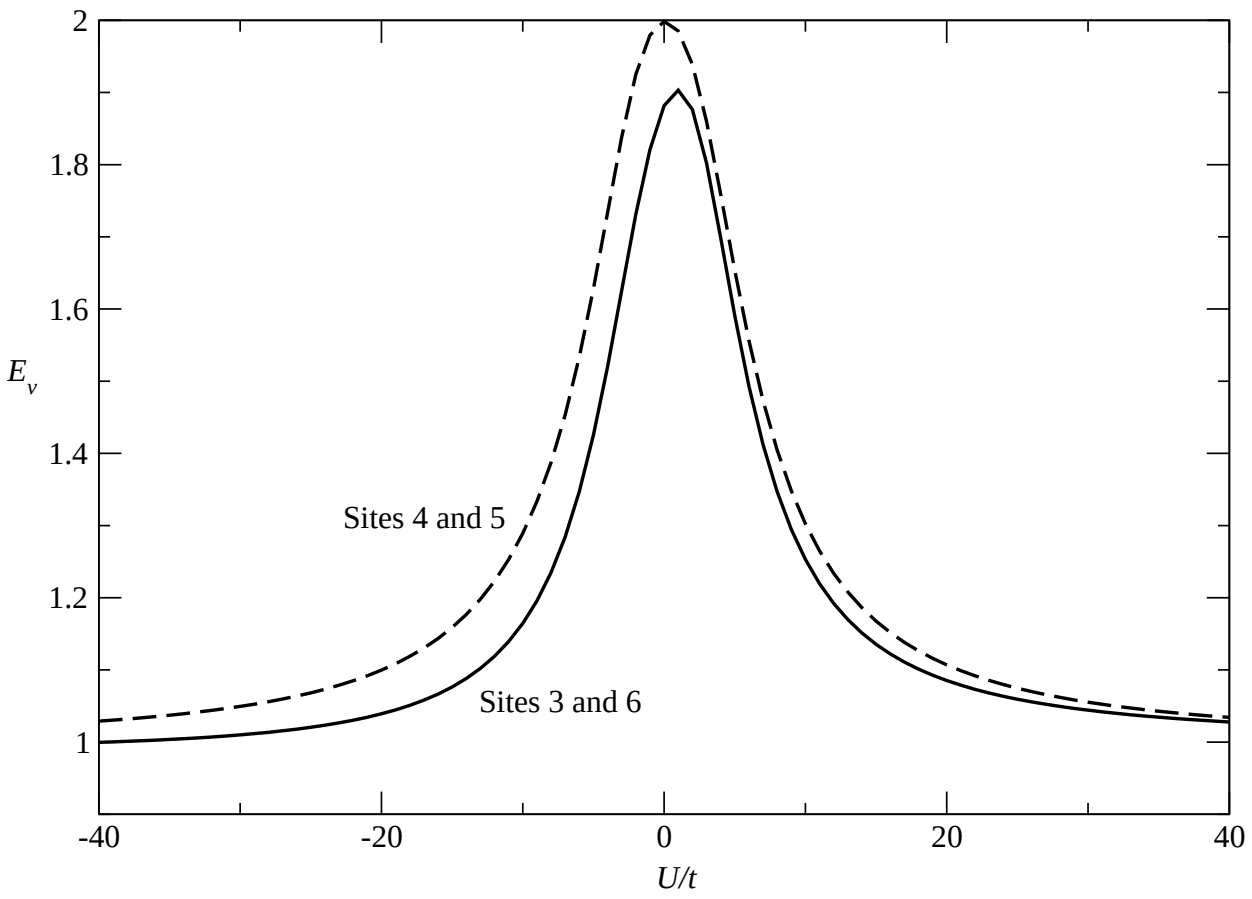

FIG. 5: Local entanglement E_v of sites 3 and 6 and sites 4 and 5 versus U/t in the asymmetric electron hopping case with $\alpha = 1000$.