Entanglement and position-space information entropy: Hubbard model as an approximation to nanostructure systems.

J. P. Coe, V. V. França, I. D’Amico

1 Department of Physics, University of York, York YO10 5DD, UK
2 Physikalisches Institut, Albert-Ludwigs-Universität, Hermann-Herder-Straße 3, D-79104 Freiburg, Germany
E-mail: jpc503@york.ac.uk, vivian.franca@physik.uni-freiburg.de, ida500@york.ac.uk

Abstract. We consider the position-space information and linear entropies as proxy measures to the average single-site entanglement—quantified using the von Neumann entropy—of the one-dimensional Hubbard model and of a one-dimensional nanostructure system comprised of an array of quantum-dots. Spatial entanglement in the quantum-dot system is also investigated via the three entropies. We appraise the use of the possible proxy measures in the Hubbard model as an approximation to their use for the nanostructure system.

1. Introduction
Systems based on quantum-dot (QD) nanostructures could be used as components for quantum information processing devices. Since entanglement is considered a key ingredient for quantum information processes, ascertaining the availability of entanglement in these nanostructures would appear to be useful when designing them. However it is often practically impossible to exactly model many-electron systems, such as complex nanostructures, and therefore precisely calculate their entanglement degree. Approximation methods such as the Hubbard model allow systems of many strongly-correlated electrons to be modelled efficiently and often capture much of the important physics. We therefore consider the one-dimensional Hubbard model (HM) as an approximation to the entanglement of a one-dimensional nanostructure model consisting of two electrons interacting via a contact interaction and confined in an array of QDs.

We first assess the position-space information and linear entropies’ ability to indicate the average single-site entanglement, as quantified by the von Neumann entropy, in the two systems: if more computationally/experimentally amenable quantities were shown to reproduce the relevant behaviour of the entanglement in these systems then they could be used for the investigation of more complex nanostructure systems. It has previously been shown [1, 2] that the position-space information entropy behaves similarly in some ways to the spatial entanglement, as measured by the von Neumann entropy, for certain parameter regimes in one- and three-dimensional systems, but does not capture all of the features of the spatial entanglement.

The average single-site entanglement of the HM [3] was found to be a good approximation to that of the QD system [4] when quantified by the von Neumann entropy. Therefore here we
investigate if this holds true for other possible entanglement indicators. By doing this we can hope to better understand if the HM is an appropriate approximation to the entanglement in a QD system with a contact interaction when other entropies, perhaps simpler than the von Neumann, are used.

2. The systems

The Hamiltonian for the QD system is

$$H = \sum_{i=1,2} \left( -\frac{1}{2} \frac{d^2}{dx_i^2} + v(x_i) \right) + C_U \delta(x_1 - x_2).$$

(1)

Here the potential \( v(x_i) \) is used to model an array of regularly spaced, identical square wells, symmetric about the origin, and defined by four quantities: \( M \) the number of wells, \( d \) the barrier width between two consecutive wells, and \( w \) and \( v_0 \) the width and depth of each well. Here we use \( v_0 = -10 \) Hartrees, \( w = 2 \ a_0 \) and \( d = 0 \) or \( d = 2 \ a_0 \), \( a_0 \) the (effective) Bohr radius. \( C_U \) controls the strength of the interaction and allows us to determine the corresponding interaction strength of the HM.

The HM Hamiltonian is

$$H = -t M \sum_{i=1}^{M} \sum_{\sigma=1,\downarrow} \left( \hat{c}_{j,\sigma}^\dagger \hat{c}_{j+1,\sigma} + \hat{c}_{j+1,\sigma}^\dagger \hat{c}_{j,\sigma} \right) + \tilde{U} \sum_{j=1}^{M} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow},$$

which we solve for two electrons and \( M \) sites, with average particle density \( n = 2/M \). We use the hopping parameter \( t \) to rescale the interaction \( \tilde{U} \) in the dimensionless interaction strength \( U = \tilde{U}/t \). We may then estimate the appropriate \( U \) for the QD system as \( U \approx \frac{\tilde{U}_w}{t_w} \) where \( \tilde{U}_w = \frac{\tilde{C}_w}{2} \int \phi_w^1(x) dx \), and \( t_w = \langle \phi_L(x) \rangle \left( \frac{1}{2} \frac{d^2}{dx^2} + v(x) \right) |\phi_R(x)\rangle \). Here \( \phi_w \) is the non-interacting, single-particle ground-state wavefunction in any one of the square wells, while \( \phi_L \) and \( \phi_R \) are two such wavefunctions situated in adjacent wells (see [4]).

3. Comparison of possible entanglement measures

We use the von Neumann entropy of the reduced density matrix, \( S = -Tr[\rho_{\text{red}} \log_2 \rho_{\text{red}}] \), to calculate the bipartite entanglement of a pure state. The reduced density matrix is obtained by tracing out one of the subsystems \( \rho_{\text{red}} = Tr_B |\psi\rangle \langle \psi| \). We compare the often computationally simpler linear entropy, \( L = 1 - Tr[\rho_{\text{red}}^2] \), with \( S \).

We consider the single-site entanglement, which quantifies how much information about the quantum state of the other sites can be obtained by measurement at a single-site \( i \). For the HM the \( \rho_{\text{red},i} \) is diagonal in the basis of occupation \([5,6] \), \( \rho_{\text{red},i} = \text{diag}[P_i(\downarrow), P_i(\uparrow), P_i(\downarrow), P_i(\uparrow), P_i(0)] \). For the QD system, wells and their surrounding barrier regions are assigned to sites so that all of space is accounted for. This also results in a diagonal \( \rho_{\text{red},i} \) (see Ref.[4]). For a system of \( M \) sites or wells, the average single-site entanglement \( S_{\text{site}} \) is then defined by the value of \( S_i \) averaged over all sites. In addition, we calculate the spatial entanglement \([1] \) of the QD system, \( S_{\text{spatial}} \). This entanglement can be thought of as quantifying how much extra information is gained upon measuring one particle’s position about the position of the remaining particle. The corresponding entropies using \( L \) instead of \( S \) are also calculated.

We also analyse the spatial and single-site position-space information entropies defined as \( I_{\text{spatial}} = -\int n(x) \log_2 n(x) dx \) and \( I_{\text{site}} = -\frac{1}{M} \sum_i n_i \log_2 n_i \). These entropies have an appealing form as they depend only on the particle density. In addition, \( I_{\text{spatial}} \) has been used to study entanglement in the Moshinsky atom \([7] \), and can be considered as an approximation to \( S_{\text{spatial}} \) where only the diagonal terms of the reduced density matrix are considered \([1] \).
**Figure 1.** Linear ($L$), von Neumann ($S$), and position-space information ($I$) entropies versus interaction strength $U$: (a) single-site entropies and (b) spatial entropies for the QD system with 4 wells $d = 2a_0$ and $d = 0$ (insets); (c) single-site entropy in the HM with 8 sites and 2 sites (inset).

We see in Fig. 1(a) that for 4 wells with wide barriers ($d = 2a_0$), $L_{\text{site}}$ is a fairly good proxy for $S_{\text{site}}$: the general trend is captured, but one small discrepancy is the absence of the maximum for small $U$ in $L_{\text{site}}$. Interestingly, $I_{\text{site}}$ behaves like $L_{\text{site}}$ so is also a fairly good approximation to $S_{\text{site}}$. For smaller barrier width, we consider the limiting case of $d = 0$ (inset of Fig. 1(a)). Here $L_{\text{site}}$ seems to be an even better approximation to $S_{\text{site}}$, and there is no maximum in both $S_{\text{site}}$ and $L_{\text{site}}$ for small $U$. $I_{\text{site}}$ is similar enough to $L_{\text{site}}$ for positive $U$ and hence $S_{\text{site}}$.

For the spatial entanglement in the QD nanostructure, Fig. 1(b), we see that the linear entropy behaves similarly to $S_{\text{spatial}}$ for any value of $d$, while the position-space information entropy fails to describe the behaviour of $S_{\text{spatial}}$ for $d = 2a_0$, for which it is more similar to the site entanglement, $S_{\text{site}}$.

For the HM with 8 sites, Fig. 1(c), $L_{\text{site}}$ and $I_{\text{site}}$ are also good approximations to the behaviour of $S_{\text{site}}$, except $I_{\text{site}}$ increases slightly at strongly negative $U$. For the HM with 2 sites (inset), $L_{\text{site}}$ and $S_{\text{site}}$ can be used interchangeably, while $I_{\text{site}}$ is null for any $U$, as the site density is frozen at $n_t = 1$. We note that for the QD system with two wells, $I_{\text{site}}$ and $I_{\text{spatial}}$ do exhibit very small changes, but the change would be indiscernible on the scale of these graphs, and we can not confidently attribute this to a physical effect rather than a numerical phenomenon.

4. Hubbard model as an approximation to the quantum-dot system

Here we compare the average single-site linear and position-space information entropies of the HM to those of a nanostructure composed of 8 wells/sites. From Fig. 2(a) we see that, for the QD system with $d = 2a_0$, the HM $L_{\text{site}}$ and $I_{\text{site}}$ are almost identical, respectively, to $L_{\text{site}}$ and $I_{\text{site}}$ of the QD.

For $d = 0$ (Fig. 2(b)), the HM $I_{\text{site}}$ is a little less accurate than for $d = 2a_0$, but still a very good approximation to the QD $L_{\text{site}}$, while $I_{\text{site}}$ for each model behaves in a very different way. Here the QD $I_{\text{site}}$ for $d = 0$ is more similar in behaviour to the spatial entanglement. This strong change in the QD $I_{\text{site}}$ when changing $d$ was also observed in the QD $I_{\text{spatial}}$ (Fig. 1(b)): by passing from $d = 0$ to $d = 2a_0$, the QD $I_{\text{spatial}}$ becomes similar in behaviour to the single-site entanglement. This leads to a very interesting conclusion: the barrier width $d$ in the QD nanostructure seems to define for which kind of entanglement the position-space information entropy can be a good entanglement indicator; spatial ($d = 0$) or site entanglement ($d = 2a_0$).

In Fig. 2(c) we also see that the behaviour of $I$ is the same whether the spatial or site form is considered. This is interesting as $I_{\text{spatial}}$ depends on the shape of the density not just the amount of density at each site, which suggests that the behaviour of $I$ is relatively insensitive...
Figure 2. Linear (L) and information (I) entropies versus interaction strength U: single-site entropy in the HM and in the QD with 8 wells, for (a) $d = 2a_0$ and (b) $d = 0$; (c) spatial and single-site information entropy in the QD with 8 wells for $d = 2a_0$ and $d = 0$. In (c) the $I_{\text{site}}$ was rescaled ($I_{\text{site}} \equiv MI_{\text{site}}$).

to the fine details of the density profile.

5. Summary
We verified that the linear entropy, in both the QD and HM systems, can reproduce qualitatively the von Neumann entropy behaviour and hence the entanglement. We found that the position-space information entropy can indicate different types of entanglement in the QD system, depending on the barrier width $d$: for $d = 2a_0$ it is a good indicator of the average single-site entanglement, while for $d = 0$ its trend is similar to the spatial entanglement. For the HM the single-site position-space information entropy indicated the general behaviour of entanglement as a function of $U$ except for the two site case.

We verified that both the single-site linear and position-space entropies in the QD nanostructure with $d = 2a_0$ can be quantitatively described by the equivalent entropy of the HM, with excellent precision. This corroborates our previous findings [4] for the von Neumann entropy. For the limit of vanishing barrier width, the linear entropy of the HM is also a good approximation to describe the entanglement in the QD system. But the information entropy in the QD for this limit seems to behave as an indicator of spatial entanglement rather than single-site entanglement.

Acknowledgments
JPC and IDA gratefully acknowledge funding from EPSRC grant EP/F016719/1. VVF is supported by Brazilian funding from CAPES.

References
[1] Coe J P, Sudbery A and D’Amico I 2008 Phys. Rev. B 77 205122
[2] Coe J P, Abdullah S and D’Amico I 2010 J. Appl. Phys. 107 09E110
[3] França V V and Capelle K 2006 Phys. Rev. A 74 042325
[4] Coe J P, França V V and D’Amico I 2010 Phys. Rev. A 81 052321
[5] Zanardi P 2002 Phys. Rev. A 65 042101
[6] Larsson D and Johansson H 2006 Phys. Rev. A 73 042320
[7] Amovilli C and March N H 2004 Phys. Rev. A 69 054302