Approximation of the entanglement in quantum dot chains using Hubbard models

J P Coe\textsuperscript{1}, V V França\textsuperscript{2}, I D’Amico\textsuperscript{1}

\textsuperscript{1} The Department of Physics, The University of York, Heslington, York, UK
\textsuperscript{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 investigate the Hubbard model, and the extended Hubbard model with and without correlated hopping, as an approximation to the average single-site (or local) entanglement of two-electron one-dimensional quantum dot chains with long range interactions. We focus on the effect of the chain length on the approximation accuracy. We also consider the particle-particle spatial entanglement of the three Hubbard models using the technique of Ref. [3] and compare the accuracy of this approximation to the numerically exact results of the nanostructure system.

1. Introduction

Systems of quantum dots are considered a feasible basis for quantum information processing and for investigating fundamental quantum mechanical properties such as entanglement. Modelling these many electron systems can by computationally difficult so approximations such as the use of lattice models are often employed. If these models could be seen to be valid for the entanglement, at least for certain parameter regions, they could be used for investigations of numerically-challenging many-electron nanostructures composed of longer chains of quantum dots. This could also pave the way for the use of density-functional techniques for lattice systems [1] thereby allowing an even more efficient approach to approximate the entanglement and appraise the suitability of quantum dot chains as components for quantum technologies.

The accuracy of the one-dimensional Hubbard model (HM) as an approximation to the average single-site entanglement of two-electrons trapped in a chain of quantum dots (QDs) was considered in Ref. [2]. This considered a contact interaction between particles and found the HM to be accurate for single-site entanglement calculations. Later, Ref. [3] considered a similar system with a more realistic long-range particle-particle interaction and a chain of four quantum dots. The accuracy of the average single-site entanglement of one-dimensional Hubbard model variants as an approximation to that of the QD structure was then appraised. The next largest term—at least for 3d transition metals—in the Coulomb interaction expansion [4] was incorporated to include nearest neighbour interactions: the extended Hubbard model (EHM). The third largest term [4], the correlated hopping (CH) term, was also considered to give the EHM+CH. In addition, in Ref. [3] a method to calculate the particle-particle spatial entanglement of the HM and EHM was also proposed. This resulted in the spatial degrees of
freedom being severely reduced to just the number of sites, yet worked relatively well as an approximation to the spatial entanglement of the QD system.

In this paper we consider the effect of the chain length on the accuracy with which the HM, EHM and EHM+CH approximates the average single-site and spatial entanglement of a one-dimensional long-range interacting quantum dot chain.

2. Models
The Hamiltonian for the quantum dot nanostructure system is

\[ H_{QD} = \sum_{i=1,2} \left( -\frac{1}{2} \frac{d^2}{dx_i^2} + v(x_i) \right) + C_U f(|x_1 - x_2|), \]

where \( v(x) \) models an array of identical, regularly spaced wells, each well representing a QD. The array is symmetric around the origin, and defined by the 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 respectively. The long range interaction is of the form (see, for example, refs. [5, 6])

\[ f(|x_1 - x_2|) = \frac{1}{\sqrt{1 + (x_1 - x_2)^2}}. \]

Here we use \( v_0 = 10 \) Hartrees, \( d = w = 2 a_0 \) and \( l = 1 a_0 \) where \( a_0 \) is the (effective) Bohr radius. We define the interaction strength as \( C_U \) and vary this to enable a useful comparison of the QD system with a variant of the Hubbard model. We solve the system using ‘exact’ diagonalization with a basis formed from 20 or 30 of the wave functions of the non-interacting system.

The Hamiltonian for the EHM+CH lattice model with dimensionless interaction strengths is

\[ H = -\sum_{i,\sigma} \left( \hat{c}^\dagger_{i,\sigma} \hat{c}_{i+1,\sigma} + \hat{c}^\dagger_{i+1,\sigma} \hat{c}_{i,\sigma} \right) + U \sum_i \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow} + U' \sum_{i,\sigma,\sigma'} \hat{n}_{i,\sigma} \hat{n}_{i+1,\sigma'} \]

\[ + t' \sum_{i,\sigma} \left( \hat{c}^\dagger_{i,\sigma} \hat{c}_{i+1,\sigma} + \hat{c}^\dagger_{i+1,\sigma} \hat{c}_{i,\sigma} \right) (\hat{n}_{i,-\sigma} + \hat{n}_{i+1,-\sigma}). \]

With \( U' = t' = 0 \) this is the HM, while for \( t' = 0 \) it reduces to the EHM. We use the procedures of Ref. [2, 3] to calculate the Hubbard parameters corresponding to \( C_U \) in the QD system and find \( U = 17865 C_U \), \( U' = 0.28 U \) and \( t' = 2 \times 10^{-5} U \). We solve the system with open boundary conditions for two particles using exact diagonalization.

3. Entanglement results
To quantify the entanglement we use the von Neumann entropy of the reduced density matrix, \( S = -Tr[\rho_{\text{red}} \log_2 \rho_{\text{red}}] \). To find the reduced density matrix we consider the system as bipartite and trace out one of the subsystems: \( \rho_{\text{red}} = Tr_B |\psi \rangle \langle \psi | \).

Firstly, we consider the single-site or local entanglement \( S_i \). This can be thought as quantifying the information gained about the quantum state of the other sites by measurement of a single-site \( i \). For the lattice system the \( \rho_{\text{red}} \) at site \( i \) is diagonal in the occupation basis \([7,8]\). \( \rho_{\text{red},i} = \text{diag} \{ P_i(\uparrow \downarrow), P_i(\downarrow \uparrow), P_i(\downarrow \downarrow), P_i(0) \} \). Here \( P_i(\uparrow \downarrow) \) is the probability of double particle occupation of site \( i \), \( P_i(\downarrow \uparrow) \) and \( P_i(\downarrow \downarrow) \) are those of single occupation, and \( P_i(0) \) is that of empty occupation. For the nanostructure system, QDs and their surrounding barrier regions are assigned to sites in such a way that all of space is accounted for. This again results in a diagonal \( \rho_{\text{red},i} \) (see Ref. [2]). We calculate the average single-site entanglement \( \langle S_{\text{site}} \rangle \) which, for a system of \( M \) sites or QDs, is defined by the value of \( S_i \) averaged over all sites.
We see in Fig. 1 that for attractive interactions $U < 0$ all of the approximations work well for the average single-site entanglement of the six quantum dot system, with the EHM and EHM+CH being a small improvement over the HM for $-50 \lesssim U \lesssim 0$. For repulsive interactions the approximation is reasonable for $U \lesssim 10$, but then the QD entanglement drops much more sharply than that of the lattice system. The use of the EHM or EHM+CH is only a small improvement over the HM but does little to reconcile the difference which is over 100% of the QD entanglement by $U \sim 300$. For eight quantum dots, Fig. 2, the situation is very similar except the entanglement of the QD system has not dropped by as much with respect to the lattice system’s entanglement by $U \sim 300$, but still the error is around 75%.

Figure 1. Average single-site entanglement quantified using $S_{\text{site}}$ plotted against the interaction strength $U$ for $M = 6$. QD system with long-range interaction, $d = w = 2 a_0$, $l = 1 a_0$, $v_0 = 10$ Hartree, $U = 17865 C_U$ (thick dashed line); HM (dotted line); EHM (thin dashed line) with $U' = 0.28 U$ and EHM+CH (circles) with $t' = 2 \times 10^{-5} U$.

Figure 2. Average single-site entanglement quantified using $S_{\text{site}}$ plotted against the interaction strength $U$ for $M = 8$. QD system with long-range interaction, $d = w = 2 a_0$, $l = 1 a_0$, $v_0 = 10$ Hartree, $U = 17865 C_U$ (thick dashed line); HM (dotted line); EHM (thin dashed line) with $U' = 0.28 U$ and EHM+CH (circles) with $t' = 2 \times 10^{-5} U$.

Let us now consider the particle-particle spatial entanglement [9], $S_{\text{spatial}}$, which can be thought of as quantifying the spatial information gained about one particle by measuring the other particle’s position. Using the procedure of Ref. [3] we can calculate the spatial entanglement for the lattice system. Here the degrees of spatial freedom have been reduced with respect to the system from, in principle, an infinite amount to simply the number of sites. We see in Figs. 3 and 4 that for $U < 0$ the spatial entanglement tends to increase with increasing magnitude of $U$ while the average single site entanglement (Figs. 1 and 2) generally decreased. For six wells we see in Fig. 3 that, similarly to the average single site entanglement, the lattice system approximation to the spatial entanglement is good for $U < 0$ with the EHM and EHM+CH offering a small improvement over the HM for $-50 \lesssim U \lesssim 0$. For $U > 0$ after an initial increase the entanglement of the QD system displays a maximum then decreases and saturates. The approximation from the Hubbard models for $U > 0$ is not as good as for $U < 0$, but better than that of the average single site entanglement particularly for large $U$. Interestingly, for $U \gtrsim 10$ the EHM and EHM+CH are a worse approximation to the spatial entanglement than the HM. Similar behaviour can be observed in the case of eight quantum dots (Fig. 4). We saw this behaviour for four quantum dots in Ref. [3] where we proposed that the spatial entanglement stemmed from the competition between the Coulomb interaction increasing the spatial correlation of the particles, and hence the entanglement, and the density being forced into the outer QDs resulting in a triplet-type state [6] with a lower entanglement. The EHM achieves the former better than the HM but neither model does much of the latter, so
the overestimation of the spatial entanglement of the QD system is worse when using the EHM.

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We noted in Ref. [3] that values of $U$ as large as $\sim 5700$ could correspond to experimentally viable quantum dots for the parameters chosen. Table 1 shows that around this value of $U$ the approximate average single-site entanglement using the EHM+CH is very different to that of the QD system and this percentage difference increases with the number of sites. In fact we can expect that, at very large $U$, the QD system for two particles approaches a situation where double occupation is excluded and almost all of the density resides in the outer QDs. This gives rise to an entanglement of $2/M$ which is indeed what we see for large enough $U$ in the cases of four [3], six and eight QDs. The EHM (+CH) are unable to alter the density to such an extent even for very large $U$, although they succeed in excluding double occupation. For EHM (+CH) we then expect to be able to approximate the large $U$ entanglement by that of a homogeneous density with zero double occupation [2], i.e.

$$S_{\text{th}}^{\text{site}} = \frac{2}{M} \log_2(M) + \left( \frac{2}{M} - 1 \right) \log_2 \left( 1 - \frac{2}{M} \right).$$

This gives 1.25 and 1.06 for six and eight QDs respectively, to be compared with the values in table. 1. Eq. 4 is then a reasonable approximation to the entanglement in the EHM (+CH) at large $U$ and supports our suggestions on the behaviour of the EHM (+CH) density.

The approximation to the spatial entanglement at this very large $U$ is better, although it still has around 20% error. Even this error though is surprisingly small when compared with that of the average single-site entanglement and bearing in mind the huge reduction in spatial degrees of freedom when moving to a lattice system.

For both the spatial and average single-site entanglement we have seen that for the parameters considered in this contribution the addition of the correlated hopping term to the EHM makes negligible difference to the accuracy of the approximation to the entanglement for six and eight QDs.

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**Figure 3.** Particle-particle spatial entanglement quantified using $S_{\text{spatial}}$ plotted against the interaction strength $U$ for $M = 6$. QD system with long-range interaction, $d = w = 2a_0$, $l = 1a_0$, $v_0 = 10$ Hartree, $U = 17865C_U$ (thick dashed line); HM (dotted line); EHM (thin dashed line) with $U' = 0.28U$ and EHM+CH (circles) with $t' = 2 \times 10^{-5}U$.

**Figure 4.** Particle-particle spatial entanglement quantified using $S_{\text{spatial}}$ plotted against the interaction strength $U$ for $M = 8$. QD system with long-range interaction, $d = w = 2a_0$, $l = 1a_0$, $v_0 = 10$ Hartree, $U = 17865C_U$ (thick dashed line); HM (dotted line); EHM (thin dashed line) with $U' = 0.28U$ and EHM+CH (circles) with $t' = 2 \times 10^{-5}U$.  

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Table 1. Table showing entanglement (average single-site and spatial) at $U = 5700$ for the EHM+CH and the nanostructure system with six and eight QDs.

|                | Six QDs | EHM+CH six sites | Eight QDs | EHM+CH eight sites |
|----------------|---------|------------------|-----------|--------------------|
| Average single-site | 0.34    | 1.19             | 0.25      | 1.01               |
| Spatial         | 1.00    | 1.26             | 1.00      | 1.22               |

4. Summary
We have investigated the approximation to the entanglement in a long-range interacting six or eight quantum dot chain by the Hubbard model and extended Hubbard model with or without correlated hopping. For the average single site entanglement we found that, for small values of $U$, the approximation was good. However the Hubbard models severely overestimated the entanglement as $U$ increased. This overestimation became worse at large $U$ as the number of dots increased. We note that even these very large $U$ values could correspond to realistic quantum dot models. The spatial entanglement was much better approximated even for large $U$ values which was especially interesting given the large number of spatial degrees of freedom discarded when approximating the QD system by a lattice model. The discrepancy between the QD system and the entanglement from the Hubbard model does not display in this case a marked dependency on the QD chain length, decreasing only slightly as the chain length increases.

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