Entanglement variations in model core-shell quantum dots

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Abstract. We model a core-shell quantum dot using a one dimensional system of two interacting electrons with a potential that can vary from one corresponding to a dot with comparable width of core and shell to one where the core well width becomes very small, but is always non-zero, while the shell becomes wide. We calculate the entanglement due to the spatial degrees of freedom and also the site or local entanglement found in a partition of the potential accessible to measurement. We quantify both using the linear entropy of the reduced density matrix. A sharp variation of the entanglement had been seen in earlier work for the transformation from a one dimensional model core-shell dot to a double dot [1]. We investigate whether the spatial entanglement and energy derivatives display any discontinuity as the core well width becomes small and if the two-electron state is always bound to the core well.

1. Introduction
Quantum dots are considered a good choice as a possible platform for the realisation of quantum information processing, which in principle would lead to significant benefits over classical information processing. This is partly due to the ability of quantum states to exhibit entanglement. We investigate the entanglement in a quantum dot model using an interacting two-electron one-dimensional system. We consider potential shapes which could correspond to core-shell dots or electrostatically gated dots. We compare the spatial entanglement with the site or local entanglement of the accessible partitions. For the latter we divide the system into three but assume that only two partitions are accessible to measurement. Furthermore, systems like this may also offer an interesting test-bed for investigating entanglement transitions in the few-particle regime [1]. Entanglement transitions—in the thermodynamic limit—have recently been linked with quantum phase transitions and shown to be able to identify them [2, 3]: in this case a non-analyticity in the entanglement as the control parameter is varied could be associated with a non-analyticity in the energy.

2. The system
The one-dimensional Hamiltonian in effective atomic units for our system reads

$$H = \sum_{i=1}^{2} \left[ -\frac{1}{2} \frac{d^2}{dx_i^2} + V(x_i, R) \right] + \delta(x_1 - x_2). \quad (1)$$

Here we model the Coulomb repulsion in one-dimension by using $\delta(x_1 - x_2)$. $V(x, R)$, is the potential characterised by an outer well of depth $-10$ Hartree and a deeper inner well of depth
−20 Hartree corresponding respectively to shell and core. The former increases whilst the latter decreases as the control parameter \( R \) increases. However, the inner well never disappears. The outer well width is \( W_{OW}(R) = 5 + R \). The inner well width varies as \( W_{IW}(R) = \left( \frac{4}{R} \right)^\gamma \) where \( \gamma = 13 \). See Fig. 1 for an illustration of the potential when \( R = 4 \ a \) where \( a \) is the Bohr radius.

We solve this system for various values of \( R \) using ‘exact’ diagonalisation with a basis comprising of the first 50 solutions to the 1D harmonic oscillator. With \( \omega \) chosen appropriately for the length scale of the system; we use \( \omega = 2 \). We then calculate quantities as a function of \( R \).

3. Bound state

We note that although a one-dimensional square well always has a bound state for one particle this may not be the case for an interacting system. We find that when we have two electrons interacting via a delta function then for a small enough inner well (\( R = 5.136 \ a \)) the ground-state energy per particle of the system is greater than the depth of the outer well (see Fig. 2). Hence the repulsion means that the state is no longer bound to the inner well.

![Figure 1. Potential for \( R = 4 \ a \) (solid line) and the partitions for the local entanglement calculation (dashed line).](image1.png)

![Figure 2. Ground-state energy of the system as a function of the control parameter \( R \). Inset: comparison with twice the depth of the outer well (dashed line).](image2.png)

4. Entanglement

We calculate the entanglement using the linear entropy of the reduced density matrix \( L = 1 - Tr\rho_{red}^2 \). We first consider the spatial entanglement [4], where the reduced density matrix is found by tracing out the spatial degrees of freedom of one of the particles \( \rho_{red} = Tr_1|\Psi\rangle\langle\Psi| \) which is then used to give \( L_{\text{spatial}} \). This entanglement quantifies how much extra information one would gain on measuring the position of one particle about the other particle’s position.

The spatial entanglement initially decreases (Fig. 3) as the inner well narrows due to the electrons being more confined and their spatial state becoming more similar to a non-entangled product state. However as the inner well continues to narrow more and more of the wavefunction spills into the outer well until the electrons become no longer bound to the inner well. In this parameter region the entanglement increases quickly as the electrons become much less confined in the wider outer well. Then the rate at which the entanglement increases diminishes and finally becomes driven by the (linear) expansion of the outer well (see also Fig. 5).

We next calculate the local or site entanglement [5, 6] which can be thought of as a measure of how much information we gain, upon measuring the occupation of a site, about the other sites. We move to a site occupation basis and partition the system into three ‘sites’: A [\( X_{\text{min}}, -1 \)], B [\(-1, 1 \)] and C [\( 1, X_{\text{max}} \)] (see Fig. 1). Here \( X_{\text{max}} = -X_{\text{min}} \), \( X_{\text{max}} \sim 36 \ a \). For the minimum value
of $R$ we consider ($R = 4 \ a$), the inner well width is at its maximum of 1. This well is centred at
the origin so our centre partition ($B$) always contains the inner well.

We may calculate the local entanglement using the linear entropy of the reduced
density matrix to give $L_{local}$. Now the reduced density matrix is found by tracing out the other two
partitions. This reduced density matrix is conveniently calculated in the site occupation basis
as $\text{diag}(P(\uparrow), P(\downarrow), P(\uparrow\downarrow), P(0))$ where $P(\chi)$ is the probability of occupation $\chi$ in the partition
of interest.

Rather than using the average local entanglement we calculate the mean local entanglement
of sites $A$ and $C$ thereby neglecting the local entanglement of site $B$. We use this to model the
local entanglement available if only these two parts of the system are accessible to measurement,
thereby introducing a spatial separation between the measurements. As the system is symmetric
about 0 the average ‘accessible’ local entanglement of partitions $A$ and $C$, is just the local
entanglement of partition $A$, i.e., $L_{local}^{\text{accessible}} = \frac{(L_{local,A} + L_{local,B})}{2} = L_{local,A}$. We see in Fig. 4
that this entanglement, similarly to the spatial entanglement, generally increases with increasing
$R$ once the inner well is small enough. We attribute this to the wavefunction spreading out and
thereby increasing the possibilities on measurement in a partition beyond simply finding it empty
all the time. So although an increase in spatial entanglement may suggest an increase in the
interaction of the system, and stronger interactions tend to reduce the local entanglement (see
for example [7]) by limiting the possibilities on measurement, here the spatial entanglement
and local entanglement of the accessible partitions behave similarly, both quickly increasing as
the wavefunction spreads into the outer well. We note that this local entanglement appears to
decrease very slightly after $R \sim 8 \ a$. This may be a small numerical inaccuracy due to the
widening outer well but finite $X_{max}$ in the definition of the partitions. Or, and potentially
more interesting, the decrease in ‘accessible’ local entanglement could signify that now that
the wavefunction has spread out to completely occupy the outer well, increasing $R$ combined with
the Coulomb interaction results in a reduction in the probability of the measurement of double
occupation in a partition. This may be worthy of further investigation.

The behaviour of this ‘accessible’ local entanglement suggests that it could be possible to
experimentally begin with a localised state which has little or no spatial entanglement nor
local entanglement accessible to measurement then adiabatically decrease the inner well and
expand the outer well thereby increasing the spatial entanglement and additionally the amount
of available local entanglement.
5. Derivatives

Previous work [1] showed that when the potential of a system similar to the one considered here splits into two wells the behaviour of the derivatives of the energy and the entanglement were suggestive of something akin to an analogue of a quantum phase transition in the few-particle regime. In this work we find that the narrowing of the well alone appears to not be enough to cause a sharp transition as both of the derivatives are smooth (see Figs. 5 and 6). However it seems that we can associate the region around the second stationary point in the entanglement derivative (Fig. 5) at $R \sim 5.1$ a with the particles no longer being bound to the inner well (see the inset of Fig. 2).

![Figure 5](image_url). Derivative of the linear entropy of the reduced density matrix (spatial entanglement) with respect to the control parameter $R$.

![Figure 6](image_url). Derivative of the ground-state energy with respect to the control parameter $R$.

6. Summary

We saw that the two interacting electrons are not always bound to the inner well as its width becomes narrow. This results in the spread of the wavefunction and an increase in entanglement.

We have shown that both the spatial and local entanglement of the ‘accessible’ partitions of the system can be varied by narrowing the width of the inner while increasing the outer well width. Interestingly the ‘accessible’ local entanglement we defined behaved similarly to the spatial entanglement with respect to the potential control parameter $R$.

We noted that for this system the derivatives of the spatial entanglement and energy did not show any discontinuity demonstrating that the entanglement and energy change with respect to $R$ is a smooth process in this system. However the derivative of the entanglement did appear to signal when the electrons were no longer bound to the inner well.

References

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