Interspecies entanglement with impurity atoms in a bosonic lattice gas

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The dynamics of impurity atoms introduced into bosonic gases in an optical lattice have generated a lot of recent interest, both in theory and experiment. We investigate to what extent measurements on either the impurity species or the majority species in these systems are affected by their interspecies entanglement. This arises naturally in the dynamics and plays an important role when we measure only one species. We explore the corresponding effects in strongly interacting regimes, using a combination of few-particle analytical calculations and Density Matrix Renormalisation group methods in one dimension. We identify how the resulting effects on impurities can be used to probe the many-body states of the majority species, and separately ask how to enter regimes where this entanglement is small, so that the impurities can be used as probes that do not significantly affect the majority species. The results are accessible in current experiments, and provide important considerations for the measurement of complex systems with using few probe atoms.

I. INTRODUCTION

The rich physics of impurity atoms introduced in to Bose gases has generated a lot of interest over the past few decades [1–3]. The resulting physics ranges from the realisation of models of open quantum systems [4–8] and mediated interactions [9] to impurity dynamics [9, 10] and broader polaronic effects [11–15], where the impurity can be described as a collective object when combined with the localised excitations it generated in the Bose gas, increasing its effective mass [2, 16, 17]. There has been a lot of recent theoretical work on these systems, applying new variational and field theory techniques to the problem across a variety of parameter regimes [18–30]. There has also been extensive experimental progress in observing polarons in Bose gases [9, 31–36], also in a strongly interacting regime [37]. The system we will investigate here relates specifically to impurities introduced into a Bose gas loaded into the lowest Bloch band of an optical lattice [38–40], which has also been realised in experiments [33, 31, 42], and recently discussed as an important example to characterise the probing of strongly correlated systems with impurity atoms [43].

We will particularly be interested in asking about the role of entanglement between the impurity atoms and the majority species. Entanglement in many-body systems [41–45] has itself generated a lot of interest in recent years, especially because of the information that can be extracted from entanglement in spatial modes, which can be used to help understand a variety of phenomena, e.g., to identify topological phases [46–49] or understand the growth of local entropy during thermalisation [50, 51]. Such entanglement in space has also been measured in experiments with cold atoms in optical lattices [52–54]. For multicomponent gases, the interplay between correlation and entanglement effects has been explored in both the Bose-Hubbard and the Hubbard model [55–57]. Recently, inter-species entanglement of the form we discuss here has been used to characterise the shift of the phase transition points in the two-component Bose Hubbard model due to interspecies interactions [58]. Interspecies entanglement could be a particularly useful tool to study situations where two species are entangled and we begin to make measurements on one of the two species, expecting to observe coherent phenomena. For example, when momentum distributions of impurity atoms are measured in some two-species experiments [32, 34] there is a notable decrease in the visibility of peaks in these momentum distributions, beyond what might be expected from an increase in the effective mass of the impurities due to the formation of a polaron. Under appropriate circumstances, there can be a significant contribution to such a decrease in visibility due to the
additional contributions from the interspecies entanglement. Especially when the ratio of particle numbers or system sizes between the majority species and the impurity atoms is not especially large, this entanglement can generate significant additional mixedness of the reduced state of a single species, which can play a role in this visibility.

As an example, in Fig. 1 we depict a two-component mixture in a lattice. In Fig. 1a, the two species are in a product state with no entanglement, as might be expected to occur in the ground state of a mixture with no interspecies interaction. If we trace over one species and ask what the reduced density operator is that describes the second species alone, we find it represents a pure state, with the atoms still delocalised, and with their momentum peaked at $p = 0$. However, in Fig. 1b, we have an initial state of perfectly correlated dimers between the two species, with dimer momentum peaked at $p = 0$. This represents an entangled state of the two species, and when we now trace over one species, the reduced density operator for the other species contains a mixture of all possible configurations, with a completely flat momentum distribution. Using numerical and analytical methods, we analyse this behaviour for different parameter regimes of both impurity and majority species particles. We find complex behaviour that exhibits particular signatures associated with the quantum phase diagram of the Bose-Hubbard model for the majority species. In this sense, understanding the impurity-majority species entanglement can be useful as an alternative route to probe the complex many-body behaviour, either by observing the impurity atoms, or by observing their effect on the state of the majority atoms. At the same time, if the impurity atoms are being used as a probe in the sense of Refs. [8, 43], it may be important to minimise direct entanglement between the species, and we analyse requirements in simple example cases to achieve this regime.

The article is organised as follows: In Sec. II we introduce the model and numerical methods we use to analyse the system. We then analyse the entanglement and momentum distributions for two particles on a lattice, one of each species, as a starting point for further investigations. In Sec. IV we present results for systems of multiple atoms on the lattice, and analyse the behaviour in parameter regimes corresponding to different quantum phases of the majority species. In Sec. V we then ask under which circumstances a single atom will become disentangled from the system to which it is coupled, and to this end we investigate cases where the impurity atoms and the majority species have different tunnelling rates in the lattice, and where the impurity atoms are confined to a fraction of the full length of the system. We then provide a conclusion and outlook in Sec. VI.

II. MODEL

We consider an ensemble of bosonic atoms loaded into the lowest band of an optical lattice. We denote the majority species as species 1, with $N_1$ atoms, and the impurity species as species 2, with $N_2 \leq N_1$ atoms. For sufficiently low temperatures and where interactions are smaller than the energy separation between Bloch bands, this situation is generally well described by a multi-species Bose-Hubbard model ($\hbar = 1$) [31],

$$H_{BH} = -\sum_{\langle i,j \rangle, \sigma} J_{\sigma} b_{\sigma, i}^\dagger b_{\sigma, j} + \sum_{\sigma} \frac{U_{\sigma}}{2} n_{\sigma, i}(n_{\sigma, i} - 1) + \sum_{l} U_{12} n_{1, l} n_{2, l},$$

where $b_{\sigma, i}^\dagger$ ($b_{\sigma, i}$) and $n_{\sigma, i}$ are the creation(annihilation) operator and number operator for species $\sigma \in \{1, 2\}$ on the $l$-th lattice site. Each species has nearest-neighbour tunnelling rate $J_{\sigma}$ and intra-species onsite interaction $U_{\sigma}$. The on-site inter-species interaction energy shift is then denoted $U_{12}$. We will generally take $J_1 = J_2 = J$ unless otherwise specified, and we usually take the same 1D lattice length $M$. In Sec. IV we will consider the impurity particles to be confined to a lattice length $M_2 \leq M$, and denote $M_1$ as the full length for the majority species.

Throughout this work we will mainly restrict our calculations to one dimension, in order to simplify the computations. But the basic principles we discuss here and the qualitative behaviour of the entanglement in different parameter regimes is expected to transfer directly to higher dimensions.

In what follows, we will use analytical methods to obtain exact results for a few atoms, and exact diagonalisation methods for small lattice sizes, especially to obtain values for the von Neumann entropy of entanglement. If we compute the reduced density matrix $\rho_{\sigma}$ for either of the two species,

$$\rho_{\sigma} = \text{Tr}_{\overline{\sigma}}(|\Psi\rangle\langle\Psi|),$$

where $|\Psi\rangle$ denotes the state of the total system, and $\overline{\sigma}$ here denotes the opposite species to $\sigma$, then the von Neumann entropy of entanglement can be computed as

$$S_{\sigma, \overline{\sigma}} = -\text{Tr}\{\rho_{\sigma} \log_2 \rho_{\sigma}\}. \quad (3)$$

Note that if the total state of the system is pure, then $S_{\sigma, \overline{\sigma}}$ is independent of the choice of $\sigma$. The entropy of the reduced density matrix for one species in this case entirely represents the entanglement between the two species. If $S_{\sigma, \overline{\sigma}} = 0$ the reduced density matrix is a pure state. This occurs when the entanglement is zero, and the total state is a product state of the two species.

As a guide to larger system behaviour, we employ mean-field methods based on the bosonic Gutzwiller ansatz [39], where the ground state of the two species
Bose-Hubbard Hamiltonian in \((\text{1})\) on an \(M\)-site chain is written as,

\[
|\psi\rangle = \prod_{l=1}^{M} \frac{f_{n_{1},n_{2}}^{(l)}}{\sqrt{n_{1}! n_{2}!}} \left( b_{1,l}^{\dagger} \right)^{n_{1}} \left( b_{2,l}^{\dagger} \right)^{n_{2}} |\text{vac}\rangle .
\] (4)

Here \(f_{n_{1},n_{2}}^{(l)}\) is the amplitude associated with different number states for each particle on the \(l\)-th site.

To provide additional information on the many-body physics beyond this, we employ density matrix renormalization group (DMRG) methods based around matrix product states \([60,61]\) to determine the ground state. In each case, we ensure that the results are properly converged in the bond dimension of the matrix product state, \(D\).

### III. TWO PARTICLES ON A 1D LATTICE

We can obtain an intuition for the behaviour we expect by considering the entanglement of two distinguishable particles in an optical lattice. Using an exact solution for the ground state of Eq. \((\text{1})\) \([62\,64]\), we can quantify how the entanglement and momentum distribution for each particle change as a function of the interaction strength between the bosons.

As a useful starting point, we consider the limiting cases. Because the ground state of a single particle on the lattice is a state with quasi-momentum \(p = 0\), for two particles the non-interacting ground state when \(U_{12} = 0\) is given by

\[
|\Psi_{\text{prod}}\rangle = \frac{1}{M} \left( \sum_{l} b_{1,l}^{\dagger} \right) \left( \sum_{l'} b_{2,l'}^{\dagger} \right) |\text{vac}\rangle .
\] (5)

When we compute the reduced density matrix, we then obtain

\[
\rho_{1} = \text{Tr}_{2} \{|\Psi_{\text{prod}}\rangle \langle \Psi_{\text{prod}}|\}
= \frac{1}{M} \left( \sum_{l} b_{1,l}^{\dagger} \right) |\text{vac}\rangle \langle \text{vac}| \left( \sum_{l'} b_{1,l'} \right) ,
\] (6)

which is a pure state, for which the resulting quasi-momentum distribution \(n(p)\) is peaked at \(p = 0\). However, if the particles are interacting such that \(|U_{12}| \gg J\), then for attractive interaction, we obtain instead

\[
|\Psi_{\text{ent}}\rangle = \frac{1}{\sqrt{M}} \sum_{l} b_{1,l}^{\dagger} b_{2,l}^{\dagger} |\text{vac}\rangle .
\] (7)

If we now compute the reduced density matrix, we then obtain

\[
\rho_{1} = \frac{1}{M} \sum_{l} \left( b_{1,l}^{\dagger} |\text{vac}\rangle \langle b_{1,l}| \right) ,
\] (8)

which is a mixed state with \(S_{\text{vN}} = \log_{2} M\). This mixed state with particles localised on each site arises in a sense because the state of the second species contains information on the locations of the state of the first species. The resulting momentum distribution is completely flat, despite the fact that the doublon momentum distribution is peaked at \(p = 0\).

To analyse the behaviour for arbitrary interaction strengths we look at the general solution for the two-particle wavefunction

\[
|\Psi_{2}\rangle = \sum_{x,y} \psi(x,y) b_{1,x}^{\dagger} b_{2,y}^{\dagger} |\text{vac}\rangle ,
\] (9)

with complex coefficients \(\psi(x,y)\). Taking periodic boundary conditions, we can separate the centre of mass \(R = (x + y)/2\) and relative \(r = x - y\) coordinates, and determine an analytical solution \([62\,64]\), for which we provide more details in Appendix \([\text{A}]\).

We show the analytical calculation for this relative wavefunction in Fig. \((\text{2}a)\). We see that the peak of the bound pair solutions becomes sharper as the interaction strength is increased. The single particle momentum distributions are shown for comparison in Fig. \((\text{2b})\), and show clearly the effect of interactions. As expected for \(U < 0\), with increasing interaction strength the two particles become more tightly bound and this leads to broadening of the single-particle momentum distribution. This lowering of the peak of the momentum distribution with increasing interaction strength is the signature of the effect of the entanglement between the two particles, and
in the rest of the article, we will use the height of the momentum peak or visibility for each species $\sigma$, $V_\sigma$, as an indicator of the change in momentum distributions.

In Fig. 2(c) we then look directly at the von Neumann entropy of entanglement. For attractive interactions ($U_{12} < 0$), the entanglement grows very sharply as a consequence of the direct pairing of the particles in position space that creates the bound state and reaches the saturation value for small $U_{12}/J$ (which is $\log_2 M$ as noted above). The entanglement in position space is generated by repulsion ($U_{12} > 0$) between the particles, which makes it energetically unfavourable for them to be present on the same lattice site. This does not provide as strong entanglement as in the attractive case, but still increased with increasing $U_{12}$, towards an asymptotic value. The visibility of the momentum distribution peak $V_1$ is shown in Fig. 2(d) and directly mirrors the behaviour of the entanglement, falling very sharply on the attractive side $U_{12} < 0$ as the particles become highly entangled and the momentum distribution for a single particle tends rapidly to a flat distribution. On the repulsive side ($U_{12} > 0$) also the slight drop of the visibility profile followed by a steady value reflects the corresponding entanglement of the particles. Below we will see analogous behaviour in the many-body case, made somewhat more complicated by the dynamics of interacting particles in the majority species.

IV. MANY BODY PROBLEM ON A LATTICE

In this section, we now investigate the interspecies entanglement in regimes where many-body dynamics play a key role. We identify the corresponding effects of interactions on the visibility of a $p = 0$ peak in the momentum distribution, and use this to understand signatures of the many-body phase diagram of the majority species in the dynamics of the impurity atoms.

A. Effects on the majority species

For each of the cases in this section, we compute the ground states of the Hamiltonian Eq. (1), which we compute using ED, DMRG, and Gutzwiller mean-field methods as discussed in Sec. III. As discussed above, we use the height of the peak of the quasi-momentum distribution per particle, denoted by $V_\sigma$, for the species $\sigma$, for visibility. Similarly the von Neumann entropy $S_{vN}$ shows the effect of entanglement between the two species. For the ED calculations (with periodic boundary condition) the lattice consists of 6 sites ($M$) and for the mean field and DMRG calculations we have used $M = 32$ and $M = 16$ respectively. In all cases the number-dominant reservoir species is at unit filling ($N_1 = M$) and the impurity species is at quarter filling ($N_2 = M/4$), except for $M = 6$ where we have taken $N_2 = M/3$.

FIG. 3. Entanglement and momentum distribution visibility for two bosonic species on a lattice, with varying majority species interactions, as a function of interspecies interactions. (a) The von Neumann entropy of entanglement between the two species, $S_{vN}$, computed with ED methods with periodic boundary conditions for $M = 6, N_1 = M, N_2 = M/3$ and $U_{12} = 32J$. (b) The visibility $V_1$ of the momentum distribution peaks for the majority species 1 as a function of interspecies interaction $U_{12}$ for a lattice chain length $M = 16$ with $N_1 = M, N_2 = M/4$ and $U_{12} = 32J$, computed using DMRG calculations with MPS bond dimension $D = 128$ for a range of $U_{12}$ values. (c) The visibility of the momentum distribution peak $V_2$ of the impurity species 2 for the same parameters as part b. (d) The visibility from mean-field calculations in a homogeneous lattice using the bosonic Gutzwiller ansatz for the same values of $U_1$ and with $M = 32$.

In Fig. 3 we show the entanglement of the species 1 in terms of the von Neumann entropy $S_{vN}$ as a function of inter-species interaction from the ED results in Fig. 3, and the visibility profiles from the DMRG calculations in Figs. 3(b,c) and mean field calculations in Fig. 3(d). We notice increase in entanglement and decrease in visibility as the inter-species interaction $U_{12}$ is increased from zero, as was seen in the previous section for the system of two bosons on an optical lattice. A change in $U_2$ does not have significant effect on the general entanglement or the visibility profiles, so we fix the value to be $U_{12} = 32J$.

When the majority species 1 particles are non-interacting ($U_1 = 0$) they are delocalised at $U_{12} = 0$ and we see a high visibility of the momentum peak at $p = 0$ in this case. When $U_{12}$ is increased, we see the decrease in the visibility, in a form that is largely familiar from the two-particle case in the previous section.

For repulsive interactions between majority atoms, we first look at $U_1 = 2J$ where the particles of species 1 are still largely delocalised at $U_{12} = 0$ as they still are in the superfluid regime of the single-species Bose-Hubbard model. The finite $U_1$ value, however, results in slight decrease of the visibility $V_1$. As $U_{12}$ is increased from zero we see similar behaviour for both the visibility and
von Neumann entropy to that seen in the $U_1 = 0$ case but now taking $U_{12} > 0$ further reduces the delocalisation of species 1 atoms. This leads to a small further decrease of visibility compared with the non-interacting case, but for $U_{12} < 0$ the decrease in visibility is correspondingly less than the $U_1 = 0$ case.

We see strong features of the many-body physics of the majority species entering the dynamics as we further increase $U_1$, so that $U_1/J$ is larger than the critical value for the Superfluid-Mott Insulator transition. For $U_1 = 8J$ we see that the visibility has a very different shape, which is characteristic now of the behaviour when the majority species is in a Mott Insulator regime for $U_{12} = 0$. We see that the visibility $V_1$ here has a minimum at zero inter-species interaction. This can be understood, because in the Mott Insulator the particles are exponentially localised at each lattice site. This results in a broadening of their momentum distributions and causes the dip in the height of the momentum peak. For low inter-species interaction the particles from the species 2 do not have sufficiently strong interactions to excite species 1 atoms out of the Mott Insulator entirely, but they do lead to some delocalisation through virtual amplitudes to create such excitations. This can also be seen in an increase of the von Neumann entropy. If we look at the $U_1 = 8J$ line in Fig. 3(b) the subsequent local maxima on the both sides of the minimum occurring at $U_{12} = 0$ happen due the increase in $U_{12}$ where the effect of the presence of a second species becomes stronger. As $U_{12}$ becomes comparable to $U_1$, the energy input due to the presence of a species 2 particle disrupts the localized phase as the energy penalty for having a double occupation of species 1 is comparable to the energy required to put two particles from the different species on a single site. Thus the species 1 particles begin to delocalise and the visibility increases substantially. However further increasing $U_{12}$ imposes a restriction on this delocalisation process which causes a drop in the visibility again.

The interplay between the different interaction parameters gives rise to some particularly interesting individual features at particular points in parameter space, most notably a surprisingly large increase in the value of the von Neumann entropy that occurs for $U_1 = 2J$ at around $U_{12} = -9J$, as can be seen in Fig. 3(a) (green line). This happens due to drastic changes in the nature of the ground states, and shows how sensitive this measure can be to such structural changes, in a regime where this cannot be detected via momentum distribution changes. Around $U_{12} = -10J$ it is energetically favourable to have all the species 1 and species 2 particles at one single site. In Fig. 3(a), this can happen in 6 possible ways as we look at a 6 site system with periodic boundary condition. On the other side of the peak-like structure, around $U_{12} = -8J$, it is energetically favourable to have the 2 of the species 2 particles on adjacent sites, and this configuration can also achieved in 6 different ways. The von Neumann entropy is therefore indeed $\log_2 6$ on both sides of the peak. Now around the peak, which is near $U_{12} = -9J$ all the 12 configurations become important and the von Neumann entropy becomes $\log_2 12$. Carrying out a Schmidt decomposition between the species reveals that the ground state is very close to a maximally entangled states with 6 almost equal singular values for $U_{12} = -10J$ and $U_{12} = -8J$, and 12 almost equal singular values for $U_{12} = -9J$. The other singular values are suppressed by at least three orders of magnitude. Looking at the energy levels of the composite system we can also see that the lowest six levels are very close to each other at $U_{12} = -10J$ and $U_{12} = -8J$ whereas there is an avoided crossing with second lowest six levels at around $U_{12} = -9J$.

For $U_1 = 32J$ the particles in species 1 are in the deep Mott insulator regime and in the range of $U_{12}$ that we are looking at here the energy input in the system by the presence of the particles of species 2 cannot affect the Mott insulator as $U_{12}$ is always much smaller than $U_1$. Since varying the interaction strength does not entangle species 1 with the other the von Neumann entropy stays at zero. The visibility of these highly site-localised species 1 particles also stays constant at a very low value which is even much smaller for the mean field treatment as we can see in Fig. 3(d). This is because in mean field treatment the spatial correlations in a Mott insulator are exactly zero and in a numerically exact treatment they fall exponentially with the distance in space.

In Fig. 4 we look more closely at visibility profile which changes from going through a maximum at zero inter-species interaction (for example, the $U_1 = 1.7J$ line in Fig. 4(a)) to a minimum (for example, the $U_1 = 2.9J$ line in Fig. 4(a)) as a function of the $U_1$ value. Here we notice the transition like feature which occurs in the regime where particles become more localised, but note that it occurs before the superfluid to Mott insulator phase transition in 1D, as it occurs at around $U_1 = 2J$ when computed using DMRG.

### B. Effects on the impurity species

In Fig. 5 we further investigate the effects on the impurity particles in the second species. As noted above, the properties of these impurity particles depend strongly on the many-body state of the species 1 particles and therefore should be affected by the choice of $U_1$ values, allowing them to be used as probes for the physics of the $U_1$ particles. The visibility of species 2 as a function of $U_{12}$ in general has a peak around $U_{12} = 0$ that decreases on each side. This peak-like structure starts broadening as we keep increasing $U_1$ starting from $U_1 = 0$. The visibility profiles are quite similar to those seen in the previous section for the system of two bosons on an optical lattice in terms of the mechanisms that create a maximum at $U_{12} = 0$ and a slower decrease for repulsive $U_{12}$. The value of the maximum visibility also follows a similar trend as a function of $U_{12}$ and falls sharply for attractive $U_{12}$ whereas it falls much slowly on the repul-
species 1 particles also stays constant at a very low value. The presence of the particles of species 2 cannot a Mott insulator regime and in the range of particles begin to delocalize and the visibility starts to disrupt the localized phase as the energy penalty becomes stronger. As subsequent local maximas on the both sides of the minimum would still favour a state with unity as site occupation the phase transition occurs at regime in 1D occurs at mann entropy is much slower here than the them to change their position in space which can be seen peak. For low inter-species interaction the particles from different species on a single site. Thus the species 1

$U_{12}$

and go to, for example, for identical parameters, computed with DMRG. However the same transition like behaviour occurs for attractive $U_{12}$, as a function of interspecies interactions, as a function of inter-species interaction $U_{12}$ for small values of $U_{2}$ and falls sharply for attractive $U_{12}$. The value of the maximum visibility also follows similar trend as a function of $U_{2}$ and falls exponentially with the spatial distance. Therefore we see a change in the behaviour of the visibility profile which is always much smaller than $U_{12}$. The other singular values are suppressed by at least three orders of magnitude. ... repulsive $U_{12}$. The value of the maximum visibility also follows similar trend as a function of $U_{2}$ and falls to completely vanish, as shown in Fig. 5(d). For a finite system (Fig. 5(b)) the visibility falls down and takes a constant value and that value decreases as we increase the system size.

Now for $U_{2} = 2J$ the visibility at $U_{12} = 0$ will be smaller than in the previous case as the impurity particles repulsively interact among themselves. This decrease in height of the visibility persists as we increase the $U_{2}$ value but not arbitrarily as we have discussed before. For small values of $U_{12}$ the visibility again remains unchanged and we also see the same localisation effect causing a drop in visibility at sufficiently high $U_{12}$ as before. The magnitude of $U_{12}$ at which the drop happens increases with increase in $U_{2}$ as the repulsion between the impurity particles also needs to be overcome. We see this for $U_{2} = 2J, 8J$ and $32J$ in Fig. 5(b).

For attractive $U_{2}$ we expect a similar plateau-like visibility profile but with much smaller values to start with (at and around $U_{12} = 0$) and we see that in Fig. 5(b) for $U_{2} = -2J$, although the plateau-like structure is hardly visible due to such small value of the peak. The value of visibility (for all the profiles) after the drop tends to go to $1/M$ which is the lower limit for the peak of a single
V. EFFECT OF THE RESERVOIR SIZE

Up to now we have looked at strong effects of entanglement between the two species. For certain applications, however, we would also like to identify regimes where this entanglement can be made small. Intuitively, we would expect this to happen when we have a large reservoir as the majority species and a few impurities. To estimate the effect of the largeness of the reservoir with non-interacting species, we can consider the two-particle problem where the impurity species 2 is confined to a small part of the lattice, with \( M_2 \) lattice sites, as opposed to the full length, \( M_1 \), and we also allow for different tunnelling rates for the two species.

In Fig. 6(a) we examine the solution to this problem, and show the characteristic differences in visibilities as a function of the ratio of the lattice sizes, and for different tunnelling rates. As can be seen in Fig. 6(a), \( V_2 \) increases steadily for smaller values of \( M_1 \) for a given \( M_2 \) and after \( M_1/M_2 = 3 \) reaches the value obtained in the absence of interactions.

In Fig. 6(b), we explore the effect of having a heavier impurity particle in the lattice system so that its tunnelling rate \( J_2 \) is smaller than \( J_1 \). In particular, we would like to find out how small \( J_2 \) should be compared to \( J_1 \), so that we can treat the tunnelling term for the impurity particles in perturbation theory. We can solve the two-particle problem perturbatively, in the limit of small \( J_2/J_1 \), and also numerically. Fig. 6(b) shows the corresponding visibilities, \( V_2 \), as solid lines found with exact diagonalisation, against \( M_1/M_2 \) for descending values of \( J_2/J_1 \). For \( J_2/J_1 = 10^{-3} \) we observe good agreement with results from perturbation theory.

We see that, consistent with our expectations, increasing the overall size of the majority species lattice while restricting to \( U_{12} > 0 \) rapidly achieves a regime where the entanglement and the effects on the visibility both become small. This effect is interestingly enhanced for equal interactions, and heavy impurities require a larger lattice for the majority species to reach the same regime.

VI. SUMMARY AND OUTLOOK

In this article we have investigated the many-body entanglement between two bosonic species in an optical lattice. We obtain signatures of many-body behaviour of the majority species in the mutual effects of the probe and the impurity species, especially on their momentum distribution. This could be used as a direct probe of the majority species, either by observation of the impurity atoms or by observation of their effects on the majority species. We have also identified regimes where the entanglement is small, which would be useful in more complex probe experiments. The interspecies entanglement could also be directly measured using interference techniques with multiple copies of the state in a quantum gas microscope, alternately performing the scheme of Refs. 50, 52, 54 for one or both atomic species.

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Appendix A: Solution for two particles on a lattice

Here we provide further details of the derivation of results for two particles on a lattice, from Sec. 11. The coefficients of the state can be written (by separating into centre of mass and relative coordinates) as

\[
\psi(x, y) = \sqrt{\frac{1}{M}} \psi(x, y),
\]

where the total number of sites, \( M = 2L + 1 \). With redefined effective tunnelling rate for the relative coordinate
\[ J_K = 2J \cos(K/2) \] and \( K \)-mode energy \( E_K \) we now have
\[ -J_K (\psi_K(r+1) + \psi_K(r-1) - 2\psi_K(r)) + U\delta_{r,0}\psi_K(r) = E_K \psi_K(r). \] (A2)

In the attractive case \((U < 0)\) the condition for a bound solution is \((E_K - 4J) < -2J_K\). Using normalization conditions and the inductive nature of Eq. (A2) we can obtain the relative wavefunction for the lowest energy bound state. If we think of Eq. (A2) as an equation describing a single particle on a lattice with indices running from \(-L\) to \(L\) then we obtain the following normalized wavefunction (for \(p = 0\) since we are looking for the lowest energy state),
\[ \psi(r) = \sqrt{\frac{1 - e^{-2q}}{1 + e^{-2q}} - 2e^{-q(M+1)}} e^{-q|r|}, \] (A3)

where \(q\) is real and is the solution of \(\cos(iq) = (4J - E) / 4J\) and the bound state energy \(E = -\sqrt{U_{12}^2 + 16J^2 + 4J}\).

In the repulsive case \((U_{12} > 0)\) the lowest energy state can be computed making use of the periodic boundary condition along with the assumption that the wavefunction reaches maximum at the boundaries. The normalized relative wavefunction is

\[ \psi(r) = \begin{cases} Ae^{ikr} + Ae^{-ikr} & : r \leq 0 \\ Ae^{-2ikr} & : r > 0 \end{cases}, \] (A4)

where \(A = (2(M + \cos(2kL)) + 2Re\left(\varepsilon^{-(M+1)k} - e^{-2ikk}/(1 - e^{-2ik})\right)^{-1/2} \) and \(k\) is given by \(\sin(kL + \pi/2) + (4J/U_{12}) \sin k = 0\). The ground state energy \(E = 4J(1 - \cos k)\).

Now we can also look at the limiting values of the single particle von Neumann entropy \(S_{\psi} = -\text{tr}(\rho_1 \log_2 \rho_1)\) where \(\rho_1\) is the single particle reduced density matrix. For the attractive case, as \(U_{12} \rightarrow -\infty\), we have \(e^n \rightarrow 0\) and \(\psi(x, y) \rightarrow \sqrt{1/M} \delta_{x,y}\). Therefore we can show \(S_{\psi} \rightarrow \log_2 M\). For the repulsive case as \(U_{12} / J \rightarrow \infty\), we have \(k \rightarrow \pi / 2L\) and \(\psi(x, y) \rightarrow \sqrt{1/M} \sin(\pi|x - y|/2L)\). In this case we have

\[ S_{\psi} \rightarrow - \sum_{x,x'} \left( \frac{1}{M} \sum_y \sin(k|x - y|) \sin(k|x' - y|) \right) \log_2 \left( \frac{1}{M} \sum_y \sin(k|x - y|) \sin(k|x' - y|) \right). \] (A5)

This is the same as the limiting result shown in Fig. 2.

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