Entanglement and the Mott insulator–superfluid phase transition in bosonic atom chains

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Abstract

We analyze the developing of bipartite and multipartite entanglement through the Mott insulator–superfluid quantum phase transition. Starting from a Mott insulator state, where a filling factor $\nu = N/M = 1$ per lattice site is considered, we derive an expression for a completely connected graph configuration of bosons and show how bipartite and multipartite entanglement evolve through the phase transition predicted in previous works. We show how, in the transition, bipartite entanglement is distributed through the system respecting monogamous relations.

1. Introduction

Entanglement is a fundamental quantum mechanical resource, playing a central role in quantum information science [1]. It has recently been recognized as a relevant quantity in many-particle systems for signaling of quantum phase transitions (QPTs) (see e.g. [2]). Under certain conditions a non-analyticity appearing in a many-particle system ground state will be signaled in any bipartite [3] and multipartite [4, 5] entanglement measure. Several spin-1/2 models have been proved to follow this feature. On the other hand, the interest in bosonic systems has increased recently due to the actual accessibility to several models in optical lattice experiments. One characteristic model that has attracted considerable attention is the Bose–Hubbard (BH) model under a Mott insulator (MI)–superfluid (SF) QPT. Concepts about QPTs in the BH model were firstly derived by Fisher et al [6], and demonstrated in a remarkable experiment by Greiner et al [7], becoming since then an intense object of investigation [8]. Some aspects of entanglement for bosonic systems have been explored for a wide variety of physical configurations [9–13]. However, at constant densities, a Berezinsky–Kosterlitz–Thouless (BKT) type QPT [14] from the SF to the MI phase at low temperatures is expected. One important question that may arise is how is this infinite order QPT is really signaled by entanglement measures.

In this paper we develop this questioning by investigating entanglement for a bosonic system under a constant density MI–SF QPT in two configurations: (i) a completely connected graph (CCG) geometry, where atomic interactions occur on-site and each atom is allowed to hop from one to any site of the whole lattice, figure 1(a). (ii) A linear chain of bosonic atoms trapped in a one-dimensional (1D) optical lattice, corresponding thus to the 1D BH model. Atomic interactions occur on-site and each atom is allowed to hop to the two neighboring sites, figure 1(b). The density, here represented by the rate between the number of atoms ($N$) and sites ($M$), is fixed at $\nu = N/M = 1$. Our analytical results are derived through the strong coupling expansion [15] over the MI phase state and allow us to infer how multipartite and bipartite entanglement can signal the phase transition and can be compared to previous numerical results [12, 13]. This perturbative approach is perfectly suited to analyze the phase transition for large $N$ where even numerical methods are demanding. Moreover for the CCG configuration we derive through a combinatorial reasoning the exact reduced one-site state, which thus can be employed for investigation of the MI–SF QPT signaling by a multipartite entanglement measure. One important and new aspect of our calculations is the distribution of entanglement through the MI–SF QPT, and the way in which the multipartite entanglement builds up through the transition. A significant interpretation is given.
by comparing the multipartite entanglement with bipartite entanglement.

### 2. Departure: MI and SF states

Starting from the Hamiltonian for bosonic atoms in an optical lattice, with the assumption that \( N \) is conserved, we obtain the following Hamiltonian [6, 8, 9],

\[
\mathcal{H} = U \sum_i N_i (N_i - 1) - J \sum_{i,j} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i),
\]

where \( U \) is the self-collision rate or the strength of the on-site repulsion of two atoms on the lattice site \( i \) as a function of the atomic mass and the s-wave scattering length, and \( J \) is understood as the hopping matrix element between sites \( i, j \). As usual \( N_i = \hat{a}_i^\dagger \hat{a}_i \) is the number operator at the lattice site \( i \), where the annihilation and creation operators \( a_i \) and \( \hat{a}_i \) obey the canonical commutation relations \([a_i, a_j^\dagger] = \delta_{i,j}\). The BH Hamiltonian consists of (1) taking the hopping term only between neighboring sites, while in the CCG configuration we consider hopping between any two sites. Calculations through mean-field theory, consistent with this last configuration, indicate the phase transition at the critical point of \( U/J = 5.8z \), where \( z = 2d \) is the number of nearest neighbors [6, 8, 9]. For a 1D optical lattice, this mean-field theory proposes a ratio \( J/U \approx 0.08 \) to the transition point. On the other hand calculations beyond the mean field [15] address \( U/J = 0.18 \) for the transition in the 1D homogeneous model. These last results help us to understand the experimental findings on phase transitions in a strongly confined 1D optical lattice developed by Stöferle et al. [16] in a strongly interacting regime. Although, in this case there is no real Mott–SF transition due to the trapping potential as remarked by Batrouni et al. [17], once there is not really a pure Mott phase. A recent proposal of an off-diagonal confinement technique [18] allows a pure Mott phase to be reached and presents experimental results corresponding to the theoretical models.

In that perspective, a recent quantum Monte Carlo calculation developed by Rigol et al. [19] shows that a ratio \( J/U = 0.28 \) for the 1D case should be expected for the unconfined case, and \( J/U = 0.18 \) for the confined situation.

In fact there are well-known solutions for the two quantum phases [15]. Deep into the SF phase the system is described by a coherent state where the probability distribution for the local occupancy of atoms on a single lattice site is Poissonian. Furthermore, this state is well described by a macroscopic wavefunction with long-range phase coherence throughout the lattice

\[
|\Psi_{\text{SF}}\rangle = \frac{1}{\sqrt{N!}} \left( \frac{1}{\sqrt{M}} \sum_{i=1}^{M} \hat{b}_i \right)^N |0\rangle.
\]

In the MI phase the fluctuations of the ground state of the system consist of localized atomic wavefunctions with a fixed number of atoms per site minimizing the interaction energy. The many-body ground state is then a product of local Fock states for each lattice site [9]

\[
|\Psi_{\text{MI}}\rangle = \frac{1}{\sqrt{N!}} \prod_{i=1}^{M} (\hat{b}_i)^{\lambda} |0\rangle.
\]

Although there is a difference between the two configurations, BH and CCG, it is known that in the thermodynamic limit, \( N \rightarrow \infty \), the inherent physics is essentially the same [15]. The mean-field approach for the BH model [6] is known to be good for high dimensional systems. This is due to the fact that the coordination number gets large and thus closer to the CCG configuration. Thus in fact the CCG configuration is the corresponding Hamiltonian model where the mean-field solutions are quantitatively exact. Experimentally it has been observed that optical lattices with a number of sites \( M \) of approximately \( 10^5 \) are sufficiently large to reflect the thermodynamical limit [7, 20]. The order parameter \( \Delta N^2 = \langle N^2 \rangle - \langle N \rangle^2 \) can be used to infer the transition from the (incompressible) MI phase, where \( \Delta N^2 = 0 \), to the (compressible) SF phase, where \( \Delta N^2 \neq 0 \). In fact, it is experimentally observed that there is a smooth change in the statistics of the distribution from Poissonian to a Fock state one when the SF–MI transition occurs in an optical lattice experiment [20].

The simplest way to investigate the evolution of entanglement through the QPT is to developed a perturbation treatment to determine the pure state of the system, departing from the MI ground state (3) and taking the hopping term as a perturbation [15]. This so-called strong coupling expansion is valid since the transition is expected to occur at \( J/U \) very small \(< 0.08\). Employing periodic boundary conditions and considering the unperturbed Hamiltonian as \( \hat{H}_0 = U \sum_i N_i (N_i - 1) \) we take \( \mathcal{W} = \lambda \sum_{i,j} (\hat{a}_i^\dagger \hat{a}_j + \hat{a}_j^\dagger \hat{a}_i) \) as a perturbation, defining \( \lambda = J/U \) as the perturbation parameter. Since we are dealing with the microcanonical ensemble the chemical potential \( \mu \) is neglected. This is reinforced by the assumption that the total density of bosons is fixed. In this sense we are following the transition along the constant density line that contours the upper-half of the Mott-lobe (see figure 2), and thus is expected to be a continuous infinite order BKT like QPTs. In our calculations the MI–SF phase transition occurs as soon as \( \lambda \) departs from 0.

### 3. Entropy as a multipartite entanglement measure

Since the system state is pure, multipartite entanglement (ME) can be detected by the reduced one-site linear entropy,
S = \frac{d}{d\lambda}(1 - \text{Tr}\rho_{N,1}^3), \text{ where } d \text{ is the dimension of the relevant Hilbert space [5] and } \rho_{N,1} \text{ is the reduced one-site state obtained through perturbation. This reduced one-site entropy will depict entanglement between the reduced site and the traced out modes. This has been shown for the reduced von Neuman entropy for interacting bosonic graphs [13]. The linear entropy employed here depicts exactly the same features of the von Neuman entropy in addition to allowing inference on fundamental moments due to its simpler form [5].}

In figure 3 the linear entropy and its derivative are plotted for a number of atoms up to 1000 for both the CCG and the BH configurations, employing a perturbation up to second order. To start up, we exemplify in figures 3(a) and (b) the two simplest situations, when \( N = M = 2 \) and 3, where the BH and the CCG configuration are indistinguishable for clear reasons. For \( \lambda \) small the system can be represented as a product of local states, with no entanglement. However, as \( \lambda \) is increased, we observe an increase of the linear entropy, stabilizing after \( \lambda \approx 0.3 \) for \( N = 3 \). This means that as the system tends to the SF phase, its state no longer is separable, and consequently the entanglement is increased. Distinct behaviors for the BH and CCG configurations occur only for \( N = M \geq 4 \), as can be viewed in figures 3(c) and (d), due to the different form of the perturbation term of the respective Hamiltonians. There a faster increase of the entropy for the CCG configuration is expected since each particular mode correlates with all other modes already in the first order perturbation step, while in the BH only the nearest neighbors are correlated. In this sense qualitatively they are equivalent but not quantitatively. In fact this is in perfect agreement with the expected mean-field solution [6], which signals the MI–SF transition for \( \lambda \) smaller than the actual observed one for the BH model. Figures 3(e) and (f) show calculations made for the BH model employing first order perturbation only, for several distinct numbers of bosons. It is important to remark that for increasing numbers of atoms the larger should be the perturbation order to correctly describe the distribution of entanglement. However, all those higher order terms are so small compared to the first order that again the change is only quantitative but not qualitative. By keeping higher order terms the values for the entropy, which are much smaller than the previous ones, would increase and the maxima of the derivatives would move slightly to the left, not changing its profile. The linear entropy characterizes very well the two phases predicted by the BH model. When \( \lambda = 0 \) we observe no entanglement between modes, characterizing the MI phase. The system behaves as independent modes distributed through the lattice with constant occupation. In the other limit, as \( \lambda \to 1 \) the state tends to be maximally entangled. This is a typical behavior of a system in the SF phase. Strictly speaking, in the real SF regime of \( \lambda = 1 \) the modes should be indistinguishable, but we consider that the lattice is kept high enough so that the concept of mode can still be applied. We remark that the linear entropy profile is very similar to the order parameter \( \Delta N^2 \) [13, 21]. Thus \( \Delta N^2 \) is indeed a witness of the ME in the system. Although we cannot make strong assumptions about the point where the phase transition occurs, given the perturbative approach, and from the fact that we are still considering a finite system, it can be inferred that the behavior of ME does not possess any discontinuity, not signaling a first order QPT. Moreover, for a BKT QPT occurring for these 1D models it is not expected that the entropy nor its derivative shows any discontinuity or divergence at constant average site occupation. Indeed in figure 3(f) the extension of the scaling of the maxima of the derivative with \( N \) tells us that the transition for \( N \to \infty \) occurs as soon as \( \lambda \) departs from 0. Even though the derivatives get sharper with increasing \( N \), nothing can be inferred from its behavior at \( N \to \infty \), if it is smooth or peaked.

Further in the text we show that the QPT is correctly signaled, as we concluded from the analysis of equation (8) from a formal derivation for the CCG model. We remark that in [13] similar results were obtained through exact diagonalization for a system up to ten sites, while in our present paper we derive analytic expressions using a perturbative method.

4. Evolution of entanglement in the CCG configuration

The high symmetry of the CCG configuration allows us to render an analytical expression for the reduced one-site state and thus for \( S \) in the CCG configuration, considering a global normalized state and employing equations (2) and (3). This last state is given by distributing \( N \) atoms in \( M \) sites, considering the occupancy number of each site as a label: \( |\psi\rangle = |\mathcal{D}\rangle = \sum \alpha_i |i\rangle \). \( \mathcal{D} \) being the combinatorial form to distinctly distribute \( N \) particles in \( M = N \) sites,

\[
\mathcal{D} = \binom{2N-1}{N_i}.
\]  

\( \alpha_i \) is a complex parameter characterizing the contribution of each combinatorial state \( |i\rangle \) in the description of the physical state \( |\psi\rangle \). It is related to the energetic cost of a given occupancy. For instance, the less costly global state is in the MI phase with one single atom occupying each site (only single occupancy): \( |1\rangle = |111 \cdots 1\rangle \), whose corresponding weight parameter is \( \alpha_1 \). Higher occupancies are energetically costly.
since the on-site interaction becomes very strong and leads to a highly unstable state as the occupancy in a determined site is increased. Thus the constraint determined by $|\alpha_i|^2 \geq |\alpha_{i+1}|^2$ must be observed. In fact, from a more fundamental point of view, $\alpha_i$ is related to the correlations of a site with the rest of the lattice. Since we deal with only two-body interaction $\alpha_i$ is thus related to two-body correlations, and obviously is a function of $\lambda$. Whether this function is continuous or not is exactly what implies the type of QPT from MI to SF. Here in our calculations, $\alpha_i$ is a truncated power series of the perturbation parameter $\lambda$. Starting from the state $|1\rangle$ above, after a combinatorial reasoning (see the appendix for a derivation for $N = 3$) and partial trace over $N - 1$ sites it is possible by induction to render the reduced one-site state for $v = 1$ for arbitrary $N$

$$\rho_{N,1} = (N - 2)! \sum \sum |\alpha_i|^2 A_{ij} f(j) f(i),$$  \hspace{1cm} (5)

where $f(N)$ is the integer partition function of $N$, i.e. the number of different ways to write down $N$, and

$$A_{ij} = \left( \sum_{\ell=0}^{N} r_{ij}^\ell \right) / \left( \prod_{\ell=0}^{N} r_{ij}^\ell \right),$$  \hspace{1cm} (6)

represents all the possible distinct arrangements in which the population term $f$ appears for writing down an occupancy with index $i$. Thus $r_{ij}^\ell$ is the number of times a number $\ell$ appears in the decomposition of $j$ in a given occupancy determined by $i$.

The accounting of the symbols for the occupancy of the sites can be easily inferred through a simple example (see the appendix for a more detailed derivation). Let $N = 3$, implying $f(3) = 3$ and the possibilities for the site occupancy are related to the states $|111\rangle$, $|012\rangle$ and $|003\rangle$ and their permutations. Thus, the only nonzero term for the first state (single occupancy) corresponding to $|111\rangle$, by fixing $i = 1$ is $r_{11}^1$, which is equal to 2. For the double occupancy corresponding to fixing $i = 2$, with state $|012\rangle$ and its permutations, the only nonzero terms are $r_{20}^0 = r_{20}^1 = 1$, $r_{20}^2 = r_{21}^2 = 1$ and $r_{20}^2 = r_{21}^2 = 1$. The last quantity of the symbols is related to $i = 3$ and the states $|003\rangle$, where we find $r_{30}^0 = r_{30}^1 = 1$ and $r_{30}^3 = 2$. From these values we find the reduced form

$$\rho_{N,1} = |\alpha_1|^2 |1\rangle \langle 1| + 2|\alpha_2|^2 |0\rangle \langle 0| + |1\rangle \langle 1| + |2\rangle \langle 2|$$  \hspace{1cm} (7)

Now the reduced one-site linear entropy, $S$, can be calculated from equation (5) and plotted in function $\lambda$ and $N$ up to the required order, as in figure 2.

Let us make some important remarks. Firstly, as we noticed before, with increasing $N$, higher orders of perturbation are required to correctly describe the state. However, from the hierarchy of $\alpha_i$ above, those higher order terms are likely to be very small, and thus a first or second order perturbation is invariably good enough for the description of the behavior of ME. This testifies to the good qualitative description given only in first order of perturbation for the BH model given previously. Secondly, we remark on the signaling of the QPT by $S$ in the thermodynamical limit $N \rightarrow \infty$ by making use of a perturbative approach. In this limit $f(N) \rightarrow \infty$ as well. Also for an infinite number of occupancies each one of the particular $|\alpha_i|$ tends to zero and more importantly $A_{ij}$ is just a constant large number. Thus the first derivative in $\lambda$ of $S$ is written as

$$\frac{\partial S}{\partial \lambda} = -2 \frac{d}{d \lambda} \sum_{i=0}^{\infty} |\alpha_i|^2 \sum_{j=0}^{\infty} A_{ij}^2 \frac{\partial |\alpha_i|^2}{\partial \lambda}.$$  \hspace{1cm} (8)

In this limit, each $i$th term in the summation is close to zero unless the derivative in $\alpha_i$ be divergent or at least very large. For a continuous QPT $\partial |\alpha_i|^2 / \partial \lambda$ would be the origin of a discontinuity or divergence if the transition is of the second order [5]. For an infinite order QPT such as the BKT although the derivative in $\alpha_i$ may be large, it is finite, but still signals the QPT as a maximal. This reasoning is valid for higher order derivatives, which are then always continuous, typical of the infinite order transition. In contrast the energy corresponding to the system perturbed state $E(\lambda) = \sum_n \lambda_n \epsilon_n^{\alpha_n}$, where $\epsilon_n^{\alpha_n}$ is the $n$-order energy, is always continuous on $\lambda$, by construction, and does not signal the QPT.

5. Distribution of bipartite entanglement

The second important point to be considered in this paper is on the distribution of bipartite entanglement. Since the evolution is governed by a two-body Hamiltonian, it seems reasonable that correlations start to build up by pairs, and the same reasoning applies to entanglement. The entropy $S$ captures all kinds of entanglement with the chosen reduced site, but does not allow us to distinguish between them. So is there any non-bipartite entanglement in the SF phase? The way to answer this question is through the relation of monogamy of entanglement [22]. It gives a bound in the way in which entanglement is distributed among many parties. Unlike classical correlation, entanglement cannot be shared with as many parties as one would wish without decreasing it with other parties.

We quantify bipartite entanglement (BE) through the negativity [23], defined as $N(\rho) = \|\rho^{TA}\|_1 - 1$, where $\|\rho^{TA}\|$ is the trace norm of the partially transposed state $\rho_{ij}^{T_A}$ of any pair of sites $[i,j]$ for the BH model. This is equivalent to the absolute value of the sum of negative eigenvalues of $\rho^{TA}$, vanishing for separable states. Although strictly necessary and sufficient only for Hilbert space dimension up to $2 \otimes 3$, in the present case it is correctly characterizing the BE for any $N$. In the simplest situation ($N = M = 2$), since the system is pure, in fact the squared negativity is equal to the one-site reduced linear entropy as there is only BE. Since we are interested in a monogamic relation [22] for distribution of bipartite entanglement [24], we employ through the following discussion the squared negativity for quantifying bipartite entanglement.

In figure 4 we plot the squared negativity and the linear entropy for $N = 3$ and 4. Since for $N = 3$ there are only nearest neighbors for any site, the $S^2$ is the same for any two sites. When $N = M = 3$, figure 4(a), $S^2$ after showing
Figure 3. (a) Reduced one-site linear entropy and (b) corresponding derivatives, as a function of $\lambda$ for $N = M = 2$ (solid line) and 3 (dotted line) for the 1D BH and the CCG configuration. (c) Reduced one-site linear entropy and (d) respective derivative, as a function of $\lambda$ for the $N = M = 4$ situation in the 1D BH (solid line) and CCG (dotted line) configurations. (e) Reduced one-site linear entropy and (f) corresponding derivative, as a function of $\lambda$ for $N = M = 10$ (solid line), 50 (dotted), 100 (triangles) and 1000 (circles) calculated up to the first order for the 1D BH configuration.

an increase in the transition, stabilizes at lower values than the one-site linear entropy. Due to translational invariance, this squared negativity when multiplied by two gives all possible bipartite entanglement with the reduced site 1. So the difference between the entropy shown in the figure and the squared negativity multiplied by two, gives what is called residual entanglement \([22, 24]\). Since here only bipartite and tripartite entanglement may occur, the residual entanglement signals that genuine tripartite entanglement does exist in the system. Indeed the ME develops through the bipartite one (the two curves evolve similarly for small $\lambda$). But as soon as tripartite entanglement starts to develop the two curves diverge from each other. We can express \([22, 24]\) this relation denoting the measure of the multipartite entanglement as $E_{123} = E_{1|2} + E_{1|3} + E_{123}$, where $E_{1|2} = E_{1|3} = \tau$ represents the bipartite entanglement, here calculated as $\tau = N^2$ and $E_{123}$ as the residual entanglement, which in this case is a genuine tripartite entanglement. Here we conclude that the genuine tripartite entanglement is equal to $E_{123} = E_{1|23} - 2\tau$, as shown by the dotted line in figure 4(a). From that we see that as soon as the bipartite entanglement starts to develop the tripartite also develops, forcing the bipartite entanglement to decrease to an almost constant value. Deep into the superfluid phase the tripartite entanglement is much higher than the sum of all bipartite entanglement.
For \( N = M = 4 \) the squared negativity shows different behavior for nearest and next-nearest neighbors, here exemplified by \( \rho_{12} \) and \( \rho_{13} \), respectively. Contrary to the spin-\( 1/2 \) model (see e.g. [5]) the next-nearest neighbor negativity cannot be neglected in comparison to the nearest neighbor one. Instead they show a peculiar behavior signaling the monogamy of entanglement. In this \( N = M = 4 \) case (figure 4(b)), the squared negativity for \( \rho_{12} \) and \( \rho_{13} \) shows that a distinct kind of BE exists. \( N_{12}^{2} \), after increasing with the entropy, it decreases as \( N_{13}^{2} \) increases (see the inset in figure 2), showing an interesting bound on the distribution of BE. Subsequently both measures stabilize to closer values. This bound on BE is typical of the limitation on the bipartite entanglement sharing imposed by the monogamy of entanglement [22] in the sense that the increasing of the \( \rho_{12} \) entanglement at the same interval where the \( \rho_{13} \) one decreases and a reciprocity maintain a constant amount of the BE. Here the difference between the ME and the two types of BE, the residual entanglement, signals both tripartite and quadripartite entanglement. This feature continues for increasing \( N \), and there is an increasing number of types of BE. The initial crossing of BE decreases with \( N \), stabilizing after a while at higher values. This is an evident manifestation of the many classes of entanglement present in the BH model. The SF phase is intermediated by a strong ME state where any mode (site) is entangled with the others in many distinct ways. Similarly to the case for \( N = M = 3 \), we can express these contributions to the distribution of the entanglement through a similar monogamic relation denoting by \( E_{1234} \) the multipartite entanglement as equal to \( E_{12} + E_{13} + E_{14} + E_{23} + E_{134} + E_{124} + E_{1234} \), where \( E_{12} = E_{13} \neq E_{14} \) are the bipartite contributions from nearest and next-nearest neighbors, here given by \( N_{12}^{2} \) and \( N_{13}^{2} \). \( E_{123} = E_{134} = E_{124} \) are the genuine tripartite entanglement and \( E_{1234} \) is the genuine four-partite entanglement. Since we do not have a good measure to distinguish the tripartite entanglement from the four-partite we do not have any information about \( E_{123}, E_{134}, E_{124} \) and \( E_{1234} \). We have only the residual entanglement \( \chi = E_{1234} - N_{12}^{2} - N_{13}^{2} - N_{14}^{2} \), which shows a similar behavior to that for \( N = 3 \).

6. Conclusion

In short, we analyzed the evolution of multipartite and bipartite entanglement along the continuous infinite order BKT-like transition for average occupation number \( \langle N \rangle = 1 \) for the CCG and 1D BH configuration of bosonic atoms trapped in an optical lattice. We described the behavior of entanglement through the MI–SF QPT predicted for these models, showing how the reduced one-site linear entropy and negativity develop. For that we considered a perturbative approach showing that it is convenient for describing entanglement features since it allows the inference of the joint evolved modes (sites) state. Clearly the CCG calculations predict a faster transition than the BH ones, which can be easily understood in terms of the higher coordination number for the first. This is expected as well from the better picture that the CCG model gives to the well known mean-field solution for the BH model [6]. Moreover we obtained a formal analytical form for the reduced one-site (mode) and consequently for its linear entropy \( S \) that allows the inference on how good this multipartite entanglement measure is, even through a perturbative approach, for inference of the QPT at the thermodynamical limit. We conclude by noticing that in this perturbative approach for the linear entropy just the diagonal elements of the whole density matrix must be taken into account, since the partial trace keeps only these terms (see equation (5)). This allowed us to infer the linear entropy behavior for large \( N \), in a first order perturbation. It represents a remarkable reduction of numerical resources for investigation of the QPT in comparison with the full Hamiltonian diagonalization. For instance, for \( N = M = 10 \), by equation (4) one must diagonalize a \( 92,378 \times 92,378 \) matrix, while through the linear entropy it involves the calculation of just 42 coefficients in the case of the CCG configuration, which can be solved by some computational method with relative simplicity.

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Appendix

As an example of the development of equation (7) for the reduced one-site state, let us illustrate the case $N = M = 3$ and afterward we show how it can be recovered from equation (7). Let us consider the MI state for $N = M = 3$: $|111⟩$. A general state satisfying the situation of constant total number $N$ and single hopping is:

$$\rho_3 = \alpha_1|111⟩ + \alpha_2(|021⟩ + |201⟩ + |120⟩ + |012⟩ + |210⟩) + \alpha_3(|300⟩ + |030⟩ + |003⟩).$$  \hspace{1cm} (9)

When we trace out any two sites we end up with the reduced one (out of three) site state

$$\rho_{3,1} = |\alpha_1|^2|1⟩⟨1| + 2|\alpha_2|^2(|0⟩⟨0| + |1⟩⟨1| + |2⟩⟨2|) + |\alpha_3|^2|3⟩⟨3|.$$  \hspace{1cm} (10)

We would like to develop this state in a general way for an arbitrary $N$ without the need to write down the explicit $N$ sites global state like (9). For that one needs to consider how the elements $\alpha$ as well as the numbers multiplying each of the allowed occupations appeared. Each alpha appeared as a signature of a distinct maximal occupation. In this simple example we had a single, a single–double (only one site with double occupation) and single–triple maximal occupation, but when $N$ is increased different kinds of occupation may appear, such as for $N = 4$, which counts with single, single–double, double–double (two sites with double occupation), single–triple and single–quadruple maximal occupation. This tells us that the state for $N = 4$ must contain $\alpha, i = 1, \ldots, 5$, and the thing gets worse for higher $N$. For $N = 5$, for example, there are $\alpha, i = 1, \ldots, 7$ distinct parameters. It turns out that those numbers of parameters are exactly the numbers of distinct forms to write an integer $N$, i.e. they are the integer partition function of $N$, $f(N)$. Now what do the numbers appearing in (10) after the reduction of (9) mean? They show how many times a given occupation appears in a specific site, bounded to the maximal given occupation of any site. After hard thinking it can be verified by induction that the right way to write down those numbers is through a combinatorial distribution in that

$$A_{ij} = \left(\sum_{\ell = 0}^{N} r_{i\ell}^j\right)/\left(\prod_{\ell = 0}^{N} r_{i\ell}^j\right),$$  \hspace{1cm} (11)

represents all the possible distinct arrangements in which the population term $j$ appears for writing down an occupancy with index $i$. Thus $r_{i\ell}^j$ is the number of times a number $\ell$ appears in the decomposition of $j$ in a given occupancy determined by $i$. After checking for larger $N$ the expression for the one reduced site (out of $N$) reads as (7).

Now checking its validity, for $N = 3$, equation (5) reads

$$\rho_{3,1} = (3 - 2)! \sum_{i=1}^{f(N)=3} |\alpha_i|^2 \sum_{j=0}^{N-3} \sum_{k=0}^{N-3} r_{ij}^k |j⟩⟨j|. \hspace{1cm} (12)$$

To develop the sums in $i$ and $j$ we remember that $f(N) = f(3) = 3$ and we must consider the states of occupancies $|111⟩$, $|012⟩$ and $|003⟩$ and all the possible permutations of these occupations in each site to get

$$\rho_{3,1} = |\alpha_1|^2 \sum_{j=0}^{N-3} \sum_{k=0}^{N-3} r_{ij}^k |j⟩⟨j| + |\alpha_2|^2 \sum_{j=0}^{N-3} \sum_{k=0}^{N-3} r_{ij}^k |j⟩⟨j| + |\alpha_3|^2 \sum_{j=0}^{N-3} \sum_{k=0}^{N-3} r_{ij}^k |j⟩⟨j|,$$  \hspace{1cm} (13)

which through the developing in $j$ reads

$$\rho_{3,1} = |\alpha_1|^2 \left(\sum_{j=0}^{N-3} r_{ij}^1 \right)|0⟩⟨0| + \sum_{j=0}^{N-3} r_{ij}^1 |1⟩⟨1| \hspace{1cm} (14a)$$

$$+ |\alpha_2|^2 \left(\sum_{j=0}^{N-3} r_{ij}^2 \right)|0⟩⟨0| + \sum_{j=0}^{N-3} r_{ij}^2 |1⟩⟨1| \hspace{1cm} (14b)$$

$$+ |\alpha_3|^2 \left(\sum_{j=0}^{N-3} r_{ij}^3 \right)|0⟩⟨0| + \sum_{j=0}^{N-3} r_{ij}^3 |1⟩⟨1| \hspace{1cm} (14c)$$

or explicitly

$$\rho_{3,1} = |\alpha_1|^2 \left(\frac{r_{i1}^0 + r_{i1}^0 + r_{i1}^0 + r_{i1}^0}{r_{i1}^0 r_{i1}^0 r_{i1}^0 r_{i1}^0}\right)|0⟩⟨0| + \frac{r_{i1}^0 + r_{i1}^0 + r_{i1}^0 + r_{i1}^0}{r_{i1}^0 r_{i1}^0 r_{i1}^0 r_{i1}^0}\right)|1⟩⟨1| \hspace{1cm} (15a)$$

$$+ |\alpha_2|^2 \left(\frac{r_{i2}^0 + r_{i2}^0 + r_{i2}^0 + r_{i2}^0}{r_{i2}^0 r_{i2}^0 r_{i2}^0 r_{i2}^0}\right)|0⟩⟨0| + \frac{r_{i2}^0 + r_{i2}^0 + r_{i2}^0 + r_{i2}^0}{r_{i2}^0 r_{i2}^0 r_{i2}^0 r_{i2}^0}\right)|1⟩⟨1| \hspace{1cm} (15b)$$

$$+ |\alpha_3|^2 \left(\frac{r_{i3}^0 + r_{i3}^0 + r_{i3}^0 + r_{i3}^0}{r_{i3}^0 r_{i3}^0 r_{i3}^0 r_{i3}^0}\right)|0⟩⟨0| + \frac{r_{i3}^0 + r_{i3}^0 + r_{i3}^0 + r_{i3}^0}{r_{i3}^0 r_{i3}^0 r_{i3}^0 r_{i3}^0}\right)|1⟩⟨1| \hspace{1cm} (15c)$$

for each $i$.
\[
\rho_{3,1} = |\alpha_1|^2 \left\{ \frac{(0 + 0 + 0 + 0)}{(010000!)} \right\} |00000000\rangle |00000000\rangle + \\
\left\{ \frac{(0 + 2 + 0 + 0)}{(002000!)} \right\} |00000001\rangle |00000001\rangle + \\
\left\{ \frac{(0 + 0 + 0 + 0)}{(000000!)} \right\} |00000002\rangle |00000002\rangle + \\
\left\{ \frac{(0 + 0 + 0 + 0)}{(000000!)} \right\} |00000003\rangle |00000003\rangle + \\
\left\{ \frac{(0 + 0 + 0 + 0)}{(000000!)} \right\} |00000004\rangle |00000004\rangle + \\
\left\{ \frac{(0 + 0 + 0 + 0)}{(000000!)} \right\} |00000005\rangle |00000005\rangle + \\
\left\{ \frac{(0 + 0 + 0 + 0)}{(000000!)} \right\} |00000006\rangle |00000006\rangle + \\
\left\{ \frac{(0 + 0 + 0 + 0)}{(000000!)} \right\} |00000007\rangle |00000007\rangle + \\
\left\{ \frac{(0 + 0 + 0 + 0)}{(000000!)} \right\} |00000008\rangle |00000008\rangle.
\]

Finally we get the simplified relation (10), and so the correct state. This can be easily extended to higher values of \(N = M\) following the considerations for \(f(N)\) and to coefficients \(i\) and \(j\).

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