Generating accessible entanglement in bosons via pair-correlated tunneling

T. J. Volkoff\textsuperscript{1} and C. M. Herdman\textsuperscript{2}

\textsuperscript{1}Department of Physics, Konkuk University, Seoul 05029, Korea
\textsuperscript{2}Department of Physics, Middlebury College, Middlebury, VT, 05753, USA

We consider an extended Bose-Hubbard model that includes pair-correlated tunneling. We demonstrate that a minimal four-mode implementation of this model exhibits a pair-correlated regime in addition to Mott insulator and superfluid regimes. We propose a low complexity variational subspace for the ground state of the system in the pair-correlated regime, which we find to be numerically exact in pure pair-tunneling limit. Additionally, we propose a parameter-free high fidelity model wave function that qualitatively captures the features of the ground state in the pair-correlated regime. Although the operationally accessible entanglement vanishes deep inside the Mott insulator and superfluid regimes due to particle number conservation, we find that in the pure pair-correlated tunneling limit the accessible entanglement entropy grows logarithmically with the number of particles. Furthermore, we demonstrate that upon application of a unitary beamsplitter operation, the pair-correlated ground state is transformed into a state with completely accessible entanglement that is not limited by super-selection rules.

I. INTRODUCTION

A variety of experimental systems of trapped strongly interacting bosons are accurately described by Bose-Hubbard (BH) model of itinerant bosons hopping between localized modes. Such quantum phases of strongly correlated systems of bosons have been experimentally shown to display such quantum properties as stable superfluid flow\textsuperscript{1}–\textsuperscript{4}, quantized circulation\textsuperscript{5, 6}, and spin-squeezing\textsuperscript{7}–\textsuperscript{10}. Additionally, strongly correlated bosonic ground states arising from Bose-Hubbard dynamics possess quantum entanglement that can be harvested for quantum circuit-based quantum information processing protocols\textsuperscript{11, 12} and quantum metrology\textsuperscript{13, 14}.

The entanglement between two subsystems of a pure quantum state $|\psi\rangle$ may be quantified by the bipartite von Neumann entanglement entropy

$$S_{VN}(|\psi\rangle) = -\text{Tr} \rho_A \log \rho_A$$

where $\rho_A$ is the reduced density matrix under a bipartition into subsystems $A$ and its complement $B$: $\rho_A = \text{Tr}_B |\psi\rangle \langle \psi|$. However, superselection rules constrain the entanglement that is operationally accessible via local operations in particle number conservation in systems of non-relativistic bosons\textsuperscript{15}–\textsuperscript{10}. Wiseman and Vaccaro defined the accessible entanglement entropy:

$$S_{acc}(|\psi\rangle) = \sum_{n=0}^{N} p_n S_{VN}(P_n |\psi\rangle / \sqrt{p_n})$$

(1)

where $P_n$ is the projection onto the subspace where $n$ particles are in the $A$ subsystem, and $p_n = \langle \psi | P_n |\psi\rangle$. Accordingly, the total entanglement entropy may be decomposed into contributions from particle number fluctuations between subsystems, $S_{\text{fuct}}(|\psi\rangle) = -\sum_{n=0}^{N} p_n \log p_n$, and the accessible entanglement: $S_{VN} = S_{\text{fuct}} + S_{\text{acc}}$\textsuperscript{17}.

In the minimal BH system with two modes, under a mode bipartition there is only a single mode in each subsystem, and thus all entanglement is due to fluctuations of particles between subsystems; correspondingly, there is no entanglement that is accessible via local operations. In fact, at least four single particle modes are required to allow for non-zero accessible entanglement necessary for meaningful entanglement distribution and concentration\textsuperscript{15}–\textsuperscript{18}. However, in both the non-interacting and strongly interacting limits of the BH model with at least four single particle modes, the accessible entanglement vanishes; specifically, the ground state in the Mott insulator regime limits to an unentangled product state, whereas in the non-interacting limit, the ground state is a Bose-Einstein condensate where all entanglement is due to fluctuations.

In this paper we demonstrate how pair-correlated dynamics can generate accessible entanglement in itinerant boson systems described by an extended BH model. We consider a minimal four mode model of $N$ spinless bosons defined by the Hamiltonian $H = H_{\text{BH}} + H_{\text{pair}}$, where $H_{\text{BH}}$ is the Bose-Hubbard Hamiltonian for four single-particle modes that represent, e.g., the sites of an optical ring lattice, and $H_{\text{pair}}$ describes pair-correlated hopping dynamics of the particles. Explicitly,

$$H = \sum_{j=0}^{3} \left[ \frac{U}{2} n_j (n_j - 1) - J \left( a_{j+1}^\dagger a_j + h.c. \right) \right. \right.$$  

$$\left. \quad - T_2 \left( a_{j+1}^2 a_j^2 + h.c. \right) \right]$$

(2)

where $a_j$ is the bosonic annihilation operator in mode $j$, $n_j = a_j^\dagger a_j$, and the first two terms corresponds to $H_{\text{BH}}$ and the third term to $H_{\text{pair}}$. All parameters $U$, $T_2$, $J$ are
Coherent pair tunneling in the presence of single-particle tunneling suppression has been observed in strongly-coupled, optical double-well systems of ultracold $^{87}$Rb [19]. For spinless bosons, pair tunneling is analogous to the superexchange phenomenon in magnetic systems [20][21]. In ultracold spinor gases of $^{87}$Rb, both pair tunneling processes and photon-assisted hyperfine superexchange can be controlled by modulation of an optical superlattice [22][24]. Singlet pair tunneling in spinor Bose gases can be treated in the same way as the analysis of pair tunneling in the present work because, e.g., $a^2_i$ and $a^+_i a^+_j$ are both $\mathfrak{su}(1, 1)$ ladder operators. Quantum coherence due to pair-correlated tunneling in many-body, two-mode bosonic systems has previously been shown to be useful for near-optimal quantum estimation of single particle tunneling amplitudes [25]. In this paper, we address how pair-correlated tunneling can generate accessible entanglement and, when combined with an implementation of a matter-wave beamsplitter, allows the conversion of fluctuation entropy into accessible entanglement.

The regime of $H$ defined by $T_2 \gg U, J$, which we call the PC (pair-correlated) regime, corresponds to an “untwisting” of the twisted superfluid phase, the latter defined by $U, J > 0, T_2 < 0$, and so named due to the alternating sign of the argument of the correlation function $\langle a^+_i a^+_j \rangle$ [26][27]. For $J = 0$, the untwisting operation that changes the sign of $T_2$ is implemented by an on-site, alternating phase shift given in Eq.(3). However, for $J \neq 0$, there is no local $U(1)$ rotation, i.e., generated by $\sum_{j=0}^3 \theta_j n_j$, that changes the sign of $T_2$ while keeping the sign of $J$ fixed. Therefore, the twisted superfluid and PC regimes are not generically connected by local operations.

To analyze the PC regime, we first identify a low-complexity subspace where the ground state in the pure pair-tunneling ($J = U = 0$) limit resides. Additionally, we introduce a parameter-free high-fidelity model wave function that quantitatively describes the ground state in the PC regime. Unlike deep in the Mott insulator and superfluid regimes, in the pure pair-tunneling limit deep inside the PC regime, we show that the ground state has non-vanishing accessible entanglement that scales as $S_{\text{sec}} \sim \log N$. By exploiting an experimentally-realizable nonlocal unitary operation, viz., a 50:50 matter wave beamsplitter that hybridizes the single particle modes, we demonstrate an “entanglement switch” that increases the coefficient of the logarithmic scaling of accessible entanglement in the ground state of the PC regime, resulting in a many-boson state with completely accessible entanglement. By demonstrating that the PC regime exhibits useful and manipulable entanglement, we establish few-mode coherent pair hopping as an elementary module for bosonic quantum information processing.

II. GROUND STATE IN THE PAIR CORRELATED REGIME

Deep in the PC regime, the ground state is well approximated by the ground state of the interaction $H_{\text{pair}}$. Unlike the Mott insulating regime ($U \gg T_2, U \gg J$) or the superfluid regime ($J \gg T_2, J \gg U$), for which the ground states are easily obtained from perturbation theory (in fact, for $T_2 = 0$ the system is solvable by algebraic Bethe ansatz [28][31]) the PC regime does not admit a clear method to obtain an analytical ground state. In fact, $H_{\text{pair}}$ can be written as

$$H_{\text{pair}} = H_R - a^2_1 a^2_2 - a^2_2 a^2_0 - a^2_3 a^2_0 - a^2_3 a^2_1,$$

where $H_R = \sum_{i,j=1}^3 a^2_i a^2_j$ is an exactly solvable Richard-son model [32]. Therefore, $H_{\text{pair}}$ can be considered as a large, nonlinear perturbation of an exactly solvable model, although the two-axis countertwisting Hamiltonian, which is the two-mode analog of $H_{\text{pair}}$, is exactly solvable [33][34].

To gain insight into the structure of the ground state of $H_{\text{pair}}$, we first note that $U^\dagger H_{\text{pair}} U = -H_{\text{pair}}$, where $U$ is the unitary transformation

$$U = \exp \left[ -i \frac{\pi}{4} (n_0 - n_1 + n_2 - n_3) \right].$$

Note that for any quantum state $\rho$ of $N$ bosons in four modes, $U \rho U^\dagger = V \rho V^\dagger$, where $V$ can be taken to be $\exp \left[ i \frac{\pi}{2} (n_1 + n_3) \right]$ or $\exp \left[ -i \frac{\pi}{2} (n_0 + n_2) \right]$. Due to this discrete antisymmetry of $H_{\text{pair}}$, we expect the ground state to obey $U^2 |\Psi_0\rangle = |\Psi_0\rangle$. Furthermore, $H_{\text{pair}}$ is invariant under the dihedral group $D_8$ generated by cyclic permutation of the modes $a_0 \rightarrow a_1 \rightarrow a_2 \rightarrow a_3 \rightarrow a_0$ and the transposition $a_0 \leftrightarrow a_2$. Notice that, by considering the action of these symmetry operations on the vector of pair annihilation operators $(a_0^2, \ldots, a_3^2)$, the full symmetry group is found to be given by the semidirect product $D_8 \rtimes \mathbb{Z}_2$. In postulating variational ansatze for the ground state of $H_{\text{pair}}$, we are motivated by the fact that quantum states that exhibit pair correlations have been used to analyze interacting bosonic systems since the early days of the quantum theory of superfluidity [35][36], and have recently been utilized to rigorously formulate a number-conserving version of the Bogoliubov theory [37][38].

We expect that the $N$-particle ground state of $H_{\text{pair}}$ is in a variational subspace that is invariant under all symmetry operations of $D_8 \rtimes \mathbb{Z}_2$. By defining $M = N/2$ and $k_\ell = 2\pi\ell/M$, we propose the following ansatze, $|\psi(\ell)\rangle$
as a variational ground state of \( H_{\text{pair}} \):

\[
|\psi(c)\rangle = \sum_{\ell=0}^{N/2} c_\ell |\varphi_\ell\rangle,
\]

\[
|\varphi_\ell\rangle = \frac{1}{N_\ell} \left( a_0^{12} + e^{ik_\ell} a_1^{12} + a_2^{12} + e^{ik_\ell} a_3^{12} \right)^M
+ \left( a_0^{12} + e^{-ik_\ell} a_1^{12} + a_2^{12} + e^{-ik_\ell} a_3^{12} \right)^M \left| 0, 0, 0, 0 \right\rangle,
\]

where \( c_\ell \) are real variational parameters, and \( |\varphi_\ell\rangle \) are normalized, but non-orthogonal states (see Appendix A for the calculation of the normalization constants \( N_\ell \)).

For \( N = 2 \), \( |\varphi_0\rangle \) is the exact ground state of \( H_{\text{pair}} \) corresponding to energy eigenvalue \( E_0 = -4 \). Similarly, for \( N = 4 \), the exact ground state (up to normalization) corresponds to \( c_0 = 1 \) and \( c_1 = -3 + 2\sqrt{2} \) with energy eigenvalue \( E_0 = -8\sqrt{2} \). Although we have not proven that the ground state of \( H_{\text{pair}} \) takes the form of Eq. (4) for all \( N \), we do not find any physically meaningful deviation of the optimal analytical state Eq. (4) from the numerically calculated ground state; Fig. 1 shows that the optimal variational state \( |\psi(c)\rangle \) has numerically perfect (up to machine precision) optimal fidelity \( F = \max_c |\langle \psi(c)|\Psi_0\rangle| \) to the pure pair-tunneling \( (U = J = 0) \) ground state \( |\Psi_0\rangle \) up to \( N = \mathcal{O}(10^5) \).

A. High fidelity model ground state

To provide additional insight into the PC regime, we analyze a unitary transformation \( V H_{\text{pair}} V^\dagger = \tilde{H}_{\text{pair}} \) that allows one to construct an approximate linear quantum dynamics for this regime. For even \( N \), the construction involves identifying the ground state subspace of \( \tilde{H}_{\text{pair}} \) with a spin-\( N/4 \) representation of \( SU(2) \) (see Appendix B). As a result, one finds that the Hamiltonian \( -\tilde{H}_{\text{pair}} \) is equivalent to the operator \( 4M J_z + F \), where \( F \) is a self-adjoint, bounded operator which is a nonlinear function of the \( su(2) \) generators \( J_x, J_y, \) and \( J_z \). If \( F \) is neglected, one obtains an unparametrized approximate ground state of \( H_{\text{pair}} \) from the \( SU(2) \) coherent state ground state of \( J_z \). The normalized approximate ground state \( |\Phi\rangle \) obtained in this way is given by

\[
|\Phi\rangle = \frac{1}{2^M \sqrt{M!}} \left[ \left( \frac{1}{\sqrt{n_0 + n_2}} \right) (a_0^{12} + a_2^{12}) + \left( \frac{1}{\sqrt{n_1 + n_3}} \right) (a_1^{12} + a_3^{12}) \right]^M |0, 0, 0, 0\rangle.
\]

We refer to \( |\Phi\rangle \) as a model ground state for \( H_{\text{pair}} \). Although the model ground state in Eq. (5) can be considered as a condensate of \( M \) pairs of particles, it is in stark contrast with pure Bose-Einstein condensate of \( N = 2M \) particles. In particular, a pure Bose-Einstein condensate has the form of \( |\omega\rangle^{N}_N \) with \( |\omega\rangle \) is a single particle state, and thus is a separable state under a particle partitioning. In contrast, Eq. (5) is non-separable under a particle partitioning. The high-fidelity nature of \( |\Phi\rangle \) is demonstrated in Fig. 1 where we find the fidelity \( |\langle \Phi|\Psi_0\rangle| \) to the numerical ground state of \( H_{\text{pair}} \) to be better than 0.99 for up to \( N = \mathcal{O}(10^3) \). Furthermore, the inset of Fig. 1 shows that the fidelity of \( |\Phi\rangle \) can be reliably extrapolated to large \( N \); for \( N = \infty \) we find the fidelity \( F_\infty \simeq 0.99256 \). In Section IV we demonstrate that the entanglement properties of \( |\Phi\rangle \) approximate those of the true ground state of \( H_{\text{pair}} \) and use (5) as a model state to semi-quantitatively analyze accessible entanglement in the PC regime without the need for performing a variational optimization.

B. Local order parameter

The one-site occupation number variance \( \langle (\Delta n_j)^2 \rangle \) can be used as a local order parameter to distinguish the three dynamical regimes of Eq. (2). Deep inside the Mott insulating regime, the variance vanishes, whereas in the superfluid regime the variance scales linearly with \( N \), approaching \( 3N/16 \) in the \( U = T_2 = 0 \) limit. In contrast, in Fig. 2 we see that \( \langle (\Delta n_j)^2 \rangle \) scales as \( \mathcal{O}(N^2) \) in the PC regime. We can understand this by considering the model ground state \( |\Phi\rangle \) for which

\[
\langle \Phi| (\Delta n_j)^2 |\Phi\rangle = \frac{1}{16} \left( \frac{N^2}{2} - N \right).
\]

Because \( H_{\text{pair}} \) is quartic in the bosonic annihilation and creation operators, one expects that the ground state energy \( |E_0(N)| \) scales as \( \mathcal{O}(N^2) \) and that a transition between superfluid and PC regime occurs in the regime \( T_2/NJ \in \mathcal{O}(1) \). The numerical values of the local particle number variance in Fig. 2 are in agreement with a
transition in this regime. To verify the ground state energy scaling of $H_{\text{pair}}$, we show in Appendix C that in the $N \to \infty$ limit, $E_0(N)/N^2 \leq -1/2$

### III. GENERATION OF ACCESSIBLE ENTANGLEMENT

We now consider the entanglement properties of the ground state $|\Psi_0\rangle$ of Eq. (2) in the pure pair-tunneling limit. We bipartition the system into neighboring pairs of modes ($\{0,1\} \cup \{2,3\}$) and quantify the entanglement between these pairs of modes with the entanglement entropy $S_{\text{N}}$ and accessible entanglement entropy $S_{\text{acc}}$. Fig. 3 shows the scaling of $S_{\text{N}}$ and $S_{\text{acc}}$ with $N$ for the both $|\Phi\rangle$ and $|\Psi_0\rangle$. For both the model ground state and the exact ground state, we find that both $S_{\text{N}}$ and $S_{\text{acc}}$ scale as $\log N$; the lines in Fig. 3 represent three parameter fits to $S = a \log N + b + c/N$; for $|\Psi_0\rangle$ we find $a_{\text{N}} \approx 1.36$ and $a_{\text{acc}} \approx 0.37$, and for $|\Phi\rangle$, $a_{\text{N}} \approx 1.37$ and $a_{\text{acc}} \approx 0.38$. We see that $|\Phi\rangle$ quantitatively captures the entanglement in the pure pair-tunneling limit. Although the majority of the entanglement is due to fluctuations between subsystems and thus inaccessible via local operations, a finite fraction of entanglement remains accessible in the large $N$ limit.

To increase the accessible entanglement, consider the unitary operator:

$$V = e^{i\frac{\pi}{2}(a_j^1a_2^1+h.c.)}e^{-i\frac{\pi}{2}(a_1^j+a_3^j+h.c.)}$$

which performs a mode transformation into the modes $c_j^1 = \sqrt{n}a_j^1\sqrt{n} = (a_j^1 + ia_j^1)/\sqrt{2}$, where $j = 2$ is understood modulo 4. With respect to the mode bipartition $\{0,1\} \cup \{2,3\}$, $V$ is a non-local operation. Such a non-local mode transformation can be implemented experimentally via, e.g., a matter wave beamsplitter. We then consider the entanglement of $|\Psi\rangle$ under the bipartition $\{0,1\} \cup \{2,3\}$ of the new modes. After the implementation of $V$, it is observed that $S_{\text{acc}} = S_{\text{N}}$ and correspondingly all entanglement is operationally accessible by local operations. Physically, this entanglement conversion is due to the absence of particle number fluctuations between the $\{0,1\}$ and $\{2,3\}$ modes; in particular, $S_{\text{fluct}} = 0$ for both $|\Phi\rangle$ and $|\Psi_0\rangle$ since $V$ maps $|\Phi\rangle$ and $|\Psi_0\rangle$ to states with exactly $N/2$ particles in each subset of modes. Additionally, the coefficient of the $\log N$ scaling of $S_{\text{acc}}$ exhibits a switch-like increase (Fig. 3) upon the operation of $V$ on the ground state $|\Psi_0\rangle$. In particular, we find that $S_{\text{acc}}(\Psi_0) = 3\log N + O(1)$

![Diagram](image-url)
ble entanglement, and furthermore results in an increase of the log $N$ scaling of the accessible entanglement $S_{\text{acc}}$ deep in the PC regime. This increase in the coefficient of the log $N$ scaling of $S_{\text{acc}}$ brought about by $\mathcal{V}$ occurs for both the exact ground state and model ground state.

IV. CONCLUSION

Through analyses of high-fidelity variational states and parameter-free approximate ground states, we have shown that accessible entanglement can be generated via pair-correlated tunneling in an extended Bose-Hubbard model. We have thus demonstrated that pair-correlated tunneling can drive many-boson systems into states with entanglement that can be locally accessed for quantum information processing protocols. Additionally, by implementing a matter wave beamsplitter, the ground state of the PC regime is transformed into a state with fully accessible entanglement, i.e., a state in which all entanglement has been concentrated into a single particle number sector. The accessible entanglement switching behavior in the four-mode system considered in this work, which is the minimal mode number for which $S_{\text{acc}} > 0$, complements recent results on using three- and four-mode bosonic models to analyze matter-wave entanglement dynamics [10] [14]. We expect that the existence of a low-complexity variational ground state subspace and high-fidelity model wavefunctions for the PC regime will stimulate further analyses of the quantum information processing capabilities of the PC regime, including the interplay with other quantum phenomena such as superfluidity [15].

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Appendix A: Normalization and inner products of the variational basis states

Here we will consider the normalization of the basis states $|\varphi_\ell\rangle$ of the variational ground-state subspace of $H_{\text{pair}}$.

Proposition. If $k_\ell \in \{0, \pi\}$, then

$$\mathcal{N}_\ell = 2^{M+1} M! \sqrt{M+1}.$$  

Proof. Let

$$|\beta_\ell\rangle = \left[\left(a_0^{\dagger 2} + e^{ik_\ell} a_1^{\dagger 2} + a_2^{\dagger 2} + e^{ik_\ell} a_3^{\dagger 2}\right)^M + \left(a_0^{\dagger 2} + e^{-ik_\ell} a_1^{\dagger 2} + a_2^{\dagger 2} + e^{-ik_\ell} a_3^{\dagger 2}\right)^M\right]|0, 0, 0, 0\rangle$$

be an unnormalized superposition of paired states. Under the action of $\mathcal{V}$ in Eq. [8] the state

$$\left(a_0^{\dagger 2} + e^{ik_\ell} a_1^{\dagger 2} + a_2^{\dagger 2} + e^{ik_\ell} a_3^{\dagger 2}\right)^M|0, 0, 0, 0\rangle$$

is transformed isometrically to

$$2^M \left(c_0^{\dagger} c_1^{\dagger} + e^{ik_\ell} c_1^{\dagger} c_3^{\dagger}\right)^M|0, 0, 0, 0\rangle.$$  

Using the binomial theorem, one finds that the states

$$|\xi_{\ell q}\rangle = \frac{1}{M! \sqrt{M+1}} \left(c_0^{\dagger 4} + e^{\pm ik_\ell} c_1^{\dagger 4} c_3^{\dagger}\right)^M|0, 0, 0, 0\rangle$$

are normalized, where $\ell \in \{0, 1, \ldots, [M/2]\}$. If $k_\ell \in \{0, \pi\}$, then

$$|\beta_\ell\rangle = 2 \left(a_0^{\dagger 2} + e^{ik_\ell} a_1^{\dagger 2} + a_2^{\dagger 2} + e^{ik_\ell} a_3^{\dagger 2}\right)^M|0, 0, 0, 0\rangle$$

gets mapped to

$$2^{M+1} \left(c_0^{\dagger} c_2^{\dagger} + e^{ik_\ell} c_1^{\dagger} c_3^{\dagger}\right)^M|0, 0, 0, 0\rangle = 2^{M+1} M! \sqrt{M+1} |\xi_\ell\rangle,$$

and, therefore,

$$|\varphi_\ell\rangle = \frac{1}{2^{M+1} M! \sqrt{M+1}} |\beta_\ell\rangle$$

is normalized.

To calculate $\mathcal{N}_\ell$ for $k_\ell \notin \{0, \pi\}$, it is necessary to calculate the inner product $\langle \xi_q | \xi_\ell \rangle$ by using the binomial theorem. For any $q \neq \ell$ the result is

$$\langle \xi_q | \xi_\ell \rangle = \frac{1}{M+1} \left[ \sum_{j=0}^M \sum_{s=0}^M \left(\begin{array}{c} M \\rangle \langle M - j \rangle \langle j, M - j, M - j, s, M - s, M - s \rangle \end{array} \right) \right]$$

$$= \frac{1}{M+1} \sum_{j=0}^M \left(\begin{array}{c} e^{ik_\ell - k_s} \langle j, M - j, s, M - s \rangle \end{array} \right)$$

$$= \frac{1}{M+1}.$$  

where $|n_0, n_1, n_2, n_3\rangle$ are Fock states in the $c_j^{\dagger}$ basis.
Now we normalize $|\beta_\ell\rangle$ for $k_\ell \notin \{0, \pi\}$. Note that $|\beta_\ell\rangle$ is transformed isometrically to

$$2^M M! \sqrt{M + 1} \left( |\xi_\ell\rangle + |\xi_{-\ell}\rangle \right)$$

under the rotation $\mathcal{V}$, and that

$$\frac{\sqrt{M + 1}}{\sqrt{2M + 4}} \left( |\xi_\ell\rangle + |\xi_{-\ell}\rangle \right)$$

is a normalized state. Therefore,

$$|\varphi_\ell\rangle = \frac{1}{2^M M! \sqrt{2M + 4}} |\beta_\ell\rangle$$

is normalized. $\square$

The inner products of the normalized states $|\varphi_\ell\rangle$, or, equivalently, their Gram matrix, are the subject of the following Proposition.

**Proposition.** If $k_\ell \in \{0, \pi\}$ and $k_r \in \{0, \pi\}$ and $\ell \neq r$, then

$$\langle \varphi_\ell | \varphi_r \rangle = \frac{1}{M + 1}.$$  

If $k_\ell \in \{0, \pi\}$ and $k_\ell \notin \{0, \pi\}$, then

$$\langle \varphi_\ell | \varphi_r \rangle = \sqrt{\frac{2}{(M + 1)(M + 2)}}. \quad (A3)$$

If $k_r \notin \{0, \pi\}$ and $k_\ell \notin \{0, \pi\}$ and $\ell \neq r$, then

$$\langle \varphi_\ell | \varphi_r \rangle = \frac{2}{M + 2}.$$  

**Proof.** We prove Eq. (A3) explicitly and note that the other inner products are proved in the same way. If $k_\ell \in \{0, \pi\}$, then

$$|\varphi_\ell\rangle = \frac{1}{2^M M! \sqrt{M + 1}} |\psi_\ell\rangle$$

gets mapped isometrically to $|\xi_\ell\rangle$ under the action of $\mathcal{V}$. If $k_r \notin \{0, \pi\}$, then

$$|\varphi_r\rangle = \frac{1}{2^M M! \sqrt{2M + 4}} |\psi_r\rangle$$

gets mapped isometrically to

$$\frac{\sqrt{M + 1}}{\sqrt{2M + 4}} \left( |\xi_r\rangle + |\xi_{-r}\rangle \right)$$

under the action of $\mathcal{V}$. Therefore, by Eq. (A2),

$$\langle \varphi_\ell | \varphi_r \rangle = \frac{\sqrt{M + 1}}{\sqrt{2M + 4}} \left( \langle \xi_\ell | \xi_r \rangle + \langle \xi_\ell | \xi_{-r} \rangle \right)$$

$$= \sqrt{\frac{2}{(M + 1)(M + 2)}}. \square$$

**Appendix B: Model ground state and approximate ground state energy**

In terms of the $c_j$ operators introduced in section III, $H_{\text{pair}}$ takes the form

$$\tilde{H}_{\text{pair}} = \mathcal{V} H_{\text{pair}} \mathcal{V}^\dagger = -4T_2 \left( c_{01}^\dagger c_1 c_3 + h.c. \right). \quad (B1)$$

Note that with $T^{(0,1)} = e^{i\frac{\pi}{2}(n_0 - n_1)}$,

$$T^{(0,1)} H_{\text{pair}} T^{(0,1)} = -\tilde{H}_{\text{pair}},$$

which implies that a local rotation (with respect to the mode bipartition $\{0, 1\} \cup \{2, 3\}$) in the $c_j$ basis can change the sign of $\tilde{H}_{\text{pair}}$. By expressing $\tilde{H}_{\text{pair}}$ as in Eq. (B1), it is clear that the algebra generated by the observables $(n_0 + n_1)$ and $(n_2 + n_3)$ (or, equivalently, by $(n_0 + n_1)$ and the identity) consists of conserved quantities. Because of the permutation symmetry of $\tilde{H}_{\text{pair}}$, the ground state of $\tilde{H}_{\text{pair}}$ lies in the $(M + 1)^2$-dimensional subspace spanned by

$$\{ |r, r - M - s, M - s\rangle \}_{r,s \in \{0, \ldots, M\}}.$$

However, the algebra generated by $(n_0 - n_2)$ and $(n_1 - n_3)$ also consists of observables that commute with $H_{\text{pair}}$. Therefore, the ground state lies in the $(M + 1)$-dimensional subspace

$$V = \{ |s, M - s, s, M - s\rangle \}_{r,s \in \{0, \ldots, M\}}.$$

From the action of $c_j$ and $c_j^\dagger$ on the symmetric Fock space, it follows that $c_{01}^\dagger c_1 c_3 |V\rangle$ is equal, as a linear operator, to the spin observable

$$\sqrt{\frac{M}{2} + J_z} J_+ \sqrt{\frac{M}{2} - J_z}$$

acting on a spin-$M/2$ representation of $\mathfrak{su}(2)$ and that $c_{01}^\dagger c_1 c_3 |V\rangle$ is equal, as a linear operator, to the spin observable

$$\sqrt{\frac{M}{2} - J_z} J_- \sqrt{\frac{M}{2} + J_z}$$

acting on the spin-$M/2$ representation. Therefore, $\tilde{H}_{\text{pair}}$
is proportional, as a linear operator, to
\[
\sqrt{\frac{M}{2} + J_z J_+} \sqrt{\frac{M}{2} - J_z} + \sqrt{\frac{M}{2} - J_z J_-} \sqrt{\frac{M}{2} + J_z} \quad (B2)
\]
acting in a spin-\(N/4\) representation of \(SU(2)\).

The unparametrized state \(|\Phi\rangle\) is derived by considering an eigenvector of \(J_x\) with eigenvalue \(M/2\), i.e., proportional to
\[
(b^\dagger_1 + b_1)^N |0,0,0,0\rangle.
\]
By noting that, e.g.,
\[
b_1^\dagger |s, M - s\rangle = \sqrt{M - s + 1} |s, M - s + 1\rangle
\]
and
\[
\left(\frac{n_1 + n_3}{2}\right)^{-\frac{1}{2}} c_1^+_1 c_{3}^+_1 |s, M - s, s, M - s\rangle = \sqrt{M - s + 1} |s, M - s + 1, s, M - s + 1\rangle,
\]
we can consider the state
\[
|\Phi\rangle = \frac{1}{M!} \left[ \left(\frac{n_0 + n_2}{2}\right)^{-\frac{1}{2}} c_{0}^+_1 c_{1}^+_1 \right]^M + \left(\frac{n_1 + n_3}{2}\right)^{-\frac{1}{2}} c_1^+_1 c_{3}^+_1 \right]^M |0,0,0,0\rangle
\]
as an unparametrized approximate ground state. Transforming back to the original \(\{n_j\}_{j=0}^{3}\) modes gives the model ground state \(|\Phi\rangle\).

To obtain a lower bound for the particle number-dependent ground state energy \(E_0(N)\) in the PC regime, one can consider the expectation of the operator given in Eq. (B2) in the state \(|J_x = -M/2\rangle\), which defines the eigenvector of \(J_x\) with eigenvalue \(-M/2\). One finds that
\[
\langle \hat{H}_{\text{pair}} | J_x = -M/2 \rangle = -2M^2 + \mathcal{O}(M).
\]
Therefore,
\[
E_0(N) \leq \langle \hat{H}_{\text{pair}} | J_x = -M/2 \rangle = \frac{1}{2} N^2 + p(N),
\]
where \(p(N)\) is a polynomial which is linear in \(N\). It follows that
\[
\lim_{N \to \infty} \frac{E_0(N)}{N^2} \leq \lim_{N \to \infty} \frac{\langle \hat{H}_{\text{pair}} | J_x = -M/2 \rangle}{N^2} = -\frac{1}{2}.
\]

Appendix C: Accessible entanglement of model and variational ground states

In the main text, the accessible entanglement of the model ground state \(S_{\text{acc}}(\mathcal{V}|\Phi\rangle)\) with respect to the \(\{0,1\} \cup \{2,3\}\) bipartition is shown to scale as \(\mathcal{O}(\log M)\).

To understand this fact, consider the expression for \(\mathcal{V}|\Phi\rangle\) in the Fock basis
\[
\mathcal{V}|\Phi\rangle = \frac{1}{2M^2} \sum_{j=0}^{M} \sqrt{\binom{M}{j}} |j, M - j, j, M - j\rangle.
\]
where the identity \(2j!! = 2^j j!\) has been used. Since for \(\mathcal{V}|\Phi\rangle\) the number of particles in each subset of modes under this bipartition are the same, \(S_{\text{Renyi}} = 0\) and \(S_{\text{acc}} = S_{\text{acc}}\). From the above expression, it is clear that \(S_{\text{acc}}(\mathcal{V}|\Phi\rangle)\) is equal to the Shannon entropy of a random variable that obeys the \(B(M, p = 1/2)\) binomial distribution:
\[
S_{\text{acc}}(\mathcal{V}|\Phi\rangle) = -\sum_{j=0}^{M} \left(\frac{M}{2M}\right) \log \left(\frac{M}{2M}\right).
\]
The analytical expression for \(S_{\text{acc}}(\mathcal{V}|\psi(c)\rangle)\) and \(S_{\text{acc}}(\mathcal{V}|\Phi\rangle)\), i.e., the accessible of the variational ground state and model ground state, respectively, in the PC regime, with respect to the \(\{0,1\} \cup \{2,3\}\) bipartition is more cumbersome and will not be shown here. However, an upper bound for the accessible entanglement of the variational state \(\mathcal{V}|\psi(c)\rangle\) can be computed by utilizing the inequality for a state \(\psi\)\n\[
S_{\text{acc}}(\mathcal{V}|\psi\rangle) \leq -\sum_{n=0}^{N} \left(\sum_{n \neq 0} \frac{p_n}{p_n} \log \left(\frac{\sum_{n \neq 0} p_n}{p_n} \right)^2\right)
\]
where the right hand side involves an average of 2nd Rényi entropies in for \(\psi\) projected onto states with definite number sector in each subsystem.

For the transformed variational ground state \(\mathcal{V}|\psi(c)\rangle\), the right-hand side of Eq. (C1) can be easily calculated for \(B\) equal to either of the partitions \(\{0,1\} \cup \{2,3\}\) and \(\{0,2\} \cup \{1,3\}\). In particular, for \(B = \{2,3\}\), making use of the relation
\[
\mathcal{V}|\psi(c)\rangle = c_0|\xi_0\rangle + c_{M/2}|\xi_{M/2}\rangle
\]
and the fact that
\[
\text{tr}_{2,3} P_n|\xi_k\rangle \langle \xi_k| P_n = \frac{\delta_{n,M}}{M+1} \sum_{j=0}^{M} e^{i(k_{j,j}-\xi_k)}|j, M-j\rangle \langle j, M-j|,
\]
gives the result

$$S_{\text{acc}}(\ket{\psi}) \leq -\log \sum_{j=0}^{M} \left( \frac{(c_0 + (-1)^j c_{M/2})^2}{M + 1} \right) + \sum_{\ell = 1}^{\lfloor M/2 \rfloor - 1} \frac{4c_{\ell} \cos(k_{\ell j}) (c_0 + (-1)^j c_{M/2})}{\sqrt{(2M + 4)(M + 1)}} + \frac{c_{\ell j} 2 \cos(k_{\ell j}) \cos(k_{\ell' j})}{M + 2} \right)^2, \quad (C2)$$

where $c_{M/2} = 0$ if $N \neq 0 \mod 4$. The same method can be used to show that $S_{N}(\mathcal{V}|\psi(c)) = 0$ for the $\{0, 2\} \cup \{1, 3\}$ partition. Furthermore, because $\mathcal{V}$ is a tensor product of beamsplitters taking $\{0, 2\} \rightarrow \{0, 2\}$ and $\{1, 3\} \rightarrow \{1, 3\}$, $S_{\text{acc}}(\psi(c))$ also vanishes for the $\{0, 2\} \cup \{1, 3\}$ bipartition. Thus we conclude that the accessible entanglement of the ground state of $H_{\text{pair}}$ in the pure pair tunneling limit vanishes when the $\{0, 2\} \cup \{1, 3\}$ bipartition is considered.

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