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Quantum Many-Body Dynamics of Coupled Double-Well Superlattices

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We propose a method for controllable generation of non-local entangled pairs using spinor atoms loaded in an optical superlattice. Our scheme iteratively increases the distance between entangled atoms by controlling the coupling between the double wells. When implemented in a finite linear chain of $2N$ atoms, it creates a triplet valence bond state with large persistency of entanglement (of the order of $N$). We also study the non-equilibrium dynamics of the one-dimensional ferromagnetic Heisenberg Hamiltonian and show that the time evolution of a state of decoupled triplets on each double well leads to the formation of a highly entangled state where short-distance antiferromagnetic correlations coexist with longer-distance ferromagnetic ones. We present methods for detection and characterization of the various dynamically generated states. These ideas are a step forward towards the use of atoms trapped by light as quantum information processors and quantum simulators.

I. INTRODUCTION

The generation and manipulation of entanglement have been identified as important requirements for quantum teleportation [1], quantum information processing [2] and quantum communication [3]. Engineering long-ranged entangled pairs in optical lattices can also have fundamental implications in the context of quantum magnetism. For example, many frustrated spin states such as spin liquid states correspond to coherent superpositions of spin singlet states [4].

Recent experiments have made progress towards generating multiparticle entanglement among an ensemble of atoms confined in optical lattices by using controlled collisions between individual neighboring atoms [5]. However, the generation of long-distance pair entanglement in systems with short-range interaction between particles (such as optical lattices) is not an easy task. In recent proposals long-distance EPR pairs [1] are generated by first creating an entangled pair of quantum particles in one location and then physically transporting one member of the pair to another location [6]. However, decoherence during the transport reduces the quality (fidelity) of the entanglement.

Our approach is based on coherent manipulations of triplet or singlet pairs of ultra-cold atoms loaded in an array of double-well potentials called superlattice [7, 8, 9]. These manipulations, applied to isolated double wells, were used for the recent observation of superexchange interactions in optical lattices [10, 11, 12]. Here we generalize these approaches to study the many-body dynamics that arises when coupling between the double wells is allowed for. We propose various schemes that result in controllable generation of multiparticle entanglement. Specifically, we first discuss a protocol that creates from a system of spinor bosonic atoms initially prepared as an array of triplet (singlet) pairs on neighboring sites, an array of long-distance triplet (singlet) pairs across the lattice. The method consists of a simple iterative swapping procedure, performed by controlling the double-well barrier height (see Fig. 1), which enables parallel generation of long-distance EPR pairs.

We find that by combining the iterative swapping procedure with the boundary effects always present in a finite linear chain, one can engineer a state in which each atom located in the right half of the superlattice is entangled with an atom in the left half. This bipartition of the system into its left and right parts exhibits maximal entanglement entropy. Similar procedures have been proposed for coherently transporting quantum information [13] and for creating bosonic cooper-like pairs [14] in optical lattices. Additionally, we show that the parallel generation of an array of EPR pairs can be useful for efficient implementation of entanglement purification schemes [15], which aim to distill the few high-fidelity entangled pairs from the numerous low-fidelity ones.

The swapping procedure described above is implemented in an array of decoupled double wells. An interesting question that naturally arises is what happens with the state if the double wells are no longer completely decoupled, but instead there exists a finite tunneling between them. The resulting dynamics goes beyond the simple two-particle physics behind the swapping procedure and the experiments which control superexchange interactions [10]. The emerging state is the consequence of many-body dynamics of a global interacting Hamiltonian and does not require manipulations on individually accessed atoms. This is a promising approach for creating new magnetic phases without explicitly processing a quantum-computer protocol. Although we believe that the phenomena we discuss here are very general, to be specific we consider in this paper a one-dimensional chain and focus on the coherent evolution of the product state of triplets or singlets in each individual double well (Fig. 1a). These are dimerized states which break translational symmetry. This choice of initial states is motivated by the fact they can be prepared in experiments [10].

Our analysis shows that the time evolution of the triplet product state leads to the formation of a magnetic state with mixed correlations and a high degree of mul-
tiparticle entanglement, where short-range antiferromagnetic and long-range ferromagnetic correlations coexist. This state can be experimentally probed by measuring the singlet-triplet populations [11] and density-density correlations after time of flight [16]. We also find total (partial) restoration of the translational (rotational) symmetry, which suggests that our final state has some type of spin liquid character. By this we mean a state with strong intrinsic fluctuations but no broken symmetries [4], what may be different from other definitions which are based on the topological order of the quantum state [17].

The time evolution of the initial singlet state also leads to the restoration of the translational symmetry and high multiparticle entanglement but in this case we do not observe the strongly mixed correlations. The dynamic state has purely antiferromagnetic character, although with an unusual behavior of long-range correlations.

The paper is organized as follows: After introducing in Sec. II the formalism and numerical techniques we use for our analysis, in Sec. III we describe the basic Hamiltonian and its possible implementation in the context of recent experiments using optical superlattices. In Sec. IV we present the swapping procedure which we refer to as a single switch dynamics and in Sec. V we discuss the idea of iterative repetition of the switch as a means to generate long-distance entangled pairs. We also study possible ways to experimentally detect such long-range correlations. In Sec. VI we relax the isolated double-well constraint and allow for a finite coupling between the double wells. Specifically, we concentrate our analysis on the many-body dynamics that emerges when both the intra- and inter-well couplings are equal and study the coherent dynamics starting from both an initially prepared triplet product state and an initially prepared singlet product state. Finally, we present our conclusions in Sec. VII.

II. THE FORMALISM

The focus of this paper is twofold. On one hand we study experimentally relevant observables which can be used to detect and characterize the dynamics of cold atoms. On the other hand we analyze properties of entanglement in the system. The propagation and redistribution of entanglement are not only important from the quantum-information perspective, but can also help to understand the quasiparticle dynamics as demonstrated recently [18]. Such properties are best discussed in terms of the entanglement entropy which corresponds to the von Neumann entropy of the reduced density matrix with respect to a bipartition into two subsystems [19]. The entanglement entropy is defined as $S = -\text{tr} (\rho \log_2 (\rho))$, where the reduced density matrix $\rho = \text{tr} |\psi(t)\rangle \langle \psi(t)|$ is the trace over the states of either of the two subsystems. For the one-dimensional systems with open boundary conditions, we will study the entanglement entropy $S_l$ of a block of size $l$ located at the edge of the chain. In the case of an infinite system we define $S_{\text{even}}$ ($S_{\text{odd}}$) as the entropy of subsystems formed by partitioning the chain at an even (odd) bond. While any product state (a state that can be represented as a tensor product of two pure subsystem states) has zero entanglement entropy, maximally entangled states at half bipartition have entanglement entropy of $S = N$.

We use both numerical and analytic techniques to study the quantum dynamics. For the numerical treatment we adopt the time-evolving block decimation algorithm (TEBD) for finite [20, 21] and periodic infinite systems [22], which uses a matrix-product state representation and a Suzuki-Trotter decomposition of the evolution operator. It retains only states with the lowest weights in the reduced density matrix, keeping the number of states $\chi$ (the dimension of the matrices) finite. Consequently, the wave-function of weakly entangled states can be handled efficiently, with the computation times of the order of $O(\chi^3 N)$.

During the time evolution $\chi$ has to be increased in order to reproduce the growing entanglement in the system. The accuracy of the method is estimated by varying both $\chi$ and the Suzuki-Trotter slicing [23]. For short and intermediate times the TEBD algorithm allows us to get very precise results, but at the moment when the entanglement entropy exceeds $\log_2 (\chi)$, the matrix-product representation becomes no longer accurate. To deal with the evolution over long periods of time ($t \rightarrow \infty$), we use exact diagonalization [24] techniques. Even though these techniques can only deal with systems with small number of lattice sites (up to 24 sites) and suffer from recurrence effects, they are relevant for realistic setups in 1D experiments [25].

III. SETUP AND PROCEDURES

A. Effective Hamiltonian

We consider a system of $2N$ ultracold bosonic atoms with two relevant hyperfine states, which we denote as $\uparrow$ and $\downarrow$, confined within a double-well superlattice with the filling factor of 1. The latter can be experimentally implemented by superimposing two independent lattices one with twice the period of the other [9, 10].

In the deep barrier regime, the vibrational energy of each well, $\hbar \omega_0$, is the largest energy scale in the system and one can restrict the dynamics to the lowest vibrational states. When restricted to the lowest band, there are three relevant energy scales: the intra-well hopping amplitude $t_{\text{in}}$, the inter-well hopping amplitude $t_{\text{out}}$ and the on-site interaction energy $U$. In the limit of large $U \gg t_{\text{in}}, t_{\text{out}}$ we are focusing on, the system is in the Mott insulating regime and the only populated states are the singly occupied ones. The spin dynamics is described by the following effective Hamiltonian, which takes into account the coupling between the differ-
ent singly occupied states by virtual particle-hole excitations \[10, 26, 27\],

\[
H_{\text{eff}} = -J_1 \sum_j S_{2j} \cdot S_{2j+1} - J_2 \sum_j S_{2j+1} \cdot S_{2j+2},
\]

with \(J_1 = 4t_{in}^2/U\) and \(J_2 = 4t_{out}^2/U\). Since experimentally \(t_{in}\) and \(t_{out}\) can be controlled independently \[11\] by adjusting the intensities of the laser beams that generate the superlattice, we will assume that both \(J_1\) and \(J_2\) can, in general, be time-dependent functions \(J_1(t), J_2(t)\). Additionally, we note that even though for bosons the sign of the coupling constants is normally positive (ferromagnetic interactions), experimentally it is also possible to change the sign to be negative \[10\].

### B. Initial state

The starting point of our analysis is a system initially prepared in an array of triplet pairs on the neighboring sites of a double-well superlattice,

\[
|\psi(t = 0)\rangle = \prod_j |t^z_{j,j+1}\rangle,
\]

\[
|t^z_{j,j+1}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_{j,j+1} + |\downarrow\rangle_{j,j+1} + 1)
\]

This state has been recently realized in the laboratory \[10\]. In this experiment, after first preparing a Mott insulator with two bosonic atoms per double well, the atoms were transferred into a triplet state configuration by using spin-changing collisions \[28\].

For the following, it is convenient to characterize the initial state as a triplet valence bond state of length 1. Although this state is a ground state of the system of independent wells, it is not an eigenstate of a system of coupled wells. Therefore, changing the couplings \(J_{1,2}\) at \(t > 0\) leads to a complicated correlated dynamics. The specific time evolution depends significantly on the ratio of the couplings \(J_1\) and \(J_2\).

### C. Switching procedures

We consider and characterize in details three specific cases:

1. Single switch: \(J_1[t > 0] = 0, J_2[t > 0] = J\).

2. Periodic switch: \(J_1[(2n + 1)t_s > t > 2nt_s] = 0, J_2[(2n + 1)t_s > t > 2nt_s] = J\) while \(J_1[(2n + 2)t_s > t > (2n + 1)t_s] = J, J_2[(2n + 2)t_s > t > (2n + 1)t_s] = 0\) with \(n = 0, 1, 2, \ldots\) and switching time \(t_s\) specified below.

3. Homogeneous switch: \(J_1[t > 0] = J_2[t > 0] = J\).

The Hamiltonian in the first two cases consists of decoupled double wells and allows a simple analytical treatment (Sections IV, V). The homogeneous switch involves the complicated many-body dynamics of the Heisenberg chain and will be analyzed using numerical tools (Section VI).

It is convenient to introduce the bond operators \[29\] which create singlet and triplet pairs at different bonds:

\[
\hat{s}^\dagger_{j,j+1} |0\rangle = |s_{j,j+1}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_j |\downarrow\rangle_{j+1} - |\downarrow\rangle_j |\uparrow\rangle_{j+1}),
\]

\[
\hat{t}^\dagger_{j,j+1} |0\rangle = |t^z_{j,j+1}\rangle,
\]

\[
\hat{t}^\dagger_{j,j+1} |0\rangle = |t^x_{j,j+1}\rangle = \frac{1}{\sqrt{2}} (|\uparrow\rangle_j |\uparrow\rangle_{j+1} - |\downarrow\rangle_j |\downarrow\rangle_{j+1}),
\]

\[
\hat{t}^\dagger_{j,j+1} |0\rangle = |t^y_{j,j+1}\rangle = \frac{i}{\sqrt{2}} (|\uparrow\rangle_j |\downarrow\rangle_{j+1} + |\downarrow\rangle_j |\uparrow\rangle_{j+1})
\]

\(|0\rangle\) denotes the state with no atoms). These operators satisfy bosonic commutation relations and the constraint

\[
\sum_{\alpha=x,y,z} \hat{t}^\dagger_{j,j+1} \hat{s}^\dagger_{j,j+1} + \hat{s}^\dagger_{j,j+1} \hat{s}_{j,j+1} = 1.
\]
which follows from the completeness of the Hilbert space of states of an individual double well. We start our analysis by studying the single switch dynamics.

**IV. SINGLE SWITCH**

In the case $J_1 = 0$ and $J_2 = J$, the evolution operator $U(t) = e^{-iHt/\hbar}$ can be written analytically. It is given by

$$U_{\text{odd}}(t) = e^{iAt} \prod_j \left[ \cos \left( \frac{J_j t}{2\hbar} \right) 1 + i \sin \left( \frac{J_j t}{2\hbar} \right) P_{2j+1,2j+2} \right],$$  

where $P_{2j+1,2j+2} = (1/2) + 2S_{2j+1} \cdot S_{2j+2}$ is the swap operator (interchanges the spins) at sites $2j + 1, 2j + 2$ and $A$ is an irrelevant phase factor equal to $-J(N + 2)/(4\hbar)$. From Eq. (6) it is clear that the evolution is periodic with the period

$$T = 2t_s, \quad Jt_s = \pi\hbar. \tag{7}$$

At times $t = (2n + 1)t_s$, the evolution operator reduces to a product of the swap operators which, upon acting on the initial state, distribute the entanglement from atoms at sites $(2j, 2j + 1)$ to atoms at $(2j + 1, 2j + 4)$, leading to the formation of a quantum state with valence bond length equal to 3 (see Fig. 1).

$$|\psi_{t=t_s}^{(1)}\rangle = \prod_j |t_x^{2j+1,2j+4}\rangle. \tag{8}$$

The effect of this redistribution on the entanglement entropy is shown on Fig. 2. We observe that while for odd bipartitions the entanglement entropy oscillates between 0 and 2, for even bipartitions $S_{\infty}^{\text{even}}$ remains constantly 1. This is consistent with the fact that for any state which can be represented as a single valence bond state the entanglement entropy is equal to the number of EPR-pairs shared by the subsystems [30] (in our case this number is 0 and 2 at $nt_s$ for the odd bipartitions and 1 for the even). The oscillation follows closely, but not exactly, the curve

$$S_{\infty}^{\text{odd}}(t) \approx 2(1 - \cos^4 \left( \frac{Jt}{2\hbar} \right)). \tag{9}$$

The singlet and triplet populations at adjacent sites are quantities that can be experimentally probed via singlet-triplet spectroscopic measurements and Stern-Gerlach techniques [11]. In terms of bond operators (see Eq. (4)) these quantities are defined as:

$$t_{\text{even}}^{x,y,z}(t) = \frac{1}{N} \sum_j \langle \psi(t)|t^{x,y,z}_{2j,2j+1}t^{x,y,z}_{2j+1,2j+2}|\psi(t)\rangle,$$

$$s_{\text{even}}(t) = \frac{1}{N} \sum_j \langle \psi(t)|s^{x}_{2j,2j+1}s^{y}_{2j+1,2j+2}|\psi(t)\rangle,$$

$$t_{\text{odd}}^{x,y,z}(t) = \frac{1}{N} \sum_j \langle \psi(t)|t^{x,y,z}_{2j+1,2j+2}t^{x,y,z}_{2j+1,2j+2}|\psi(t)\rangle,$$

$$s_{\text{odd}}(t) = \frac{1}{N} \sum_j \langle \psi(t)|s^{x}_{2j+1,2j+2}s^{y}_{2j+1,2j+2}|\psi(t)\rangle.$$

Using the evolution operator (6), the singlet-triplet populations can be shown to evolve as

$$t_{\text{even}}^{x}(t) = \frac{1}{4} \left( 1 + 3 \cos^4 \left( \frac{Jt}{2\hbar} \right) \right), \tag{10}$$

$$t_{\text{odd}}^{x,y}(t) = s_{\text{even}}(t) = \frac{1}{4} \left( 1 - \cos^4 \left( \frac{Jt}{2\hbar} \right) \right),$$

$$t_{\text{odd}}^{x,y,z}(t) = s_{\text{odd}}(t) = \frac{1}{4}.$$

The coherence of the singlet-triplet oscillations can help to characterize the quality of the dynamical evolution. These measurements, however, are only local and do not give any indication of the distance between the entangled atoms generated at $t = (2n + 1)t_s$. The latter, on the other hand, can be probed by measuring density-density correlations of the expanding cloud or noise correlations [16]

$$G(Q(r),Q'(r')) = \frac{\sum_{\sigma\sigma'}\left< \hat{n}_{Q(r)}^{\sigma}\hat{n}_{Q'(r')}^{\sigma'} \right>}{\sum_{\sigma\sigma'}\left< \hat{n}_{Q(r)}^{\sigma}\right>\left< \hat{n}_{Q'(r')}^{\sigma'} \right> - 1}. \tag{11}$$
where $\hat{n}^\sigma_{Q(r)}$ is the atom number operator for the component $\sigma$ at position $r$ after time of flight. $G(Q(r), Q'(r'))$ is directly related to the momentum-momentum correlations of the atomic cloud at the release time, $t_R$. Deep in the Mott insulator regime $G(Q(r), Q'(r'))$ can be rewritten in terms of spin operators as

$$G(q, t_R) = \langle \psi(t_R)| \frac{1}{2N^2} \sum_{i \neq j} e^{iqa(i-j)} \left( \frac{1}{4} + \mathbf{S}_i \cdot \mathbf{S}_j \right) |\psi(t_R)\rangle = \frac{1}{2} \delta_{q,0} + \Delta(q, t_R),$$

where $q = Q - Q'$ and $a$ is the lattice spacing (Fig. 1). While the first term in Eq. (12) reproduces the interference peaks at reciprocal lattice vectors characteristic of the Mott insulator state (due to the bunching of the bosons), the second term $\Delta(q, t_R)$ provides additional information about the spin order in the system. For example, if the system is released exactly at times $t_R = nt_s$ when it is in a valence bond state of length $l$ (here $l = 1, 3$), $\Delta(q, t_R)$ will exhibit spatial oscillations with periodicity dictated by the distance between the entangled atoms (see Fig. 3)

$$\Delta(q, t_R = nt_s) = \frac{1}{4N} [1 + \cos(qa)].$$

We note that the factor $N$ in the denominator originates from the short-range character of the interactions and therefore the entanglement is only shared between pairs. It limits the applicability of noise correlations as a suitable experimental probe in systems with large number of atoms. However, the $1/N$ factor should not be a problem in current 1D systems with approximately 20 atoms per tube [25].

V. PERIODIC SWITCH

A. Generic case

We now consider the iterative sequence of switching off and on the couplings $J_1, J_2$ every $t_s$. One might think that if at time $t_s$ one reverses the couplings from $J_1 = 0, J_2 = J$ to $J_1 = J, J_2 = 0$, the dynamics will just return the state into its original form, i.e. from Eq. (8) to Eq. (2); however, this does not happen. On the contrary, as a result of the evolution under the swap operators, atoms separated by four lattice sites become now connected by triplet valence bonds and so, at the time $t = 2t_s$, the state evolves into a valence bond state with...
The successive repetition of the switching procedure leads to the propagation of the entanglement across the lattice and after \( n \) switches, performed at times \( kt_s \) (\( k = 1, \ldots, n \)), one obtains entangled pairs with length \( 2n + 1 \).

In the experimentally relevant case of an open chain, the sequential incrementation of the length of the entangled pairs is stopped when one member of the pair reaches the boundary of the lattice. The pair is then reflected and continues moving through the lattice with its length remaining unchanged. Consequently, when after \( N - 1 \) switches the pair initially located at the center of the lattice reaches the boundary, a particular state that has the maximal possible length of entangled pairs is formed. While for an odd number of double wells it corresponds to a state with an EPR-pair connecting the edges of the chain,

\[
|\psi_{t=2s}^{(2)}\rangle = \prod_j |t_{2j+5}^2\rangle.
\]

Moreover, the \( |\psi_{t=Nt_s}^{(N-1)}\rangle \) state is an eigenstate of the \( N \)-th switching operator, \( |\psi_{t=(N-1)t_s} = |\psi_{t=Nt_s}\rangle \) and thus after \( 2N \) switches the state will be rolled back to the initial nearest-neighbor triplet-product state. This property can be useful for experimentally probing the state and quantifying the fidelity of the procedure. For example, by measuring the quality of the triplet product state after \( 2N \) switches one can get information about errors that occurred during the swapping process.

We also note that even though we focused on the case of an initial array of triplet pairs, similar considerations hold if instead of triplets one starts with singlets or changes the sign of the coupling constants (as it would be in the case of fermions).

In addition, our swapping procedure can also be used for transporting a particular state of an atom without directly moving the particles: If we initially prepare all the atoms in the same state, say \( \downarrow \), except for the atom at site \( i \) which we prepare in state \( \uparrow \), after \( n \) periodic switches the state \( \uparrow \) will be transferred to the atom located at site \( i+n \).

The long-range entanglement produced by the switching procedure can be experimentally probed by noise-correlation measurements. Although for finite lattices the expected ideal pattern of well-defined peaks at \( t = nt_s \) (see Eq. (12)) changes to one with less regular structure due to the distribution of different valence bond lengths, Fig. 4 shows that it still contains relevant information such as the formation of well-defined peaks at \( q = 0 \) and \( q = \pi/a \) when the distance between entangled atoms becomes maximal.

C. Non-ideal conditions

Up to this point we have assumed that Eq. (1) accurately describes the many-body dynamics. However, defects such as holes or doubly occupied sites will make this assumption invalid.

We should emphasize that there is one particular condition which makes the entanglement generation possible despite the presence of holes. Namely, this occurs when the single-particle tunneling time is engineered to be commensurate with \( t_s \). However, if this condition is not satisfied, in general the holes will hinder the generation of long-distance entangled pairs and they should be suppressed for example by implementing additional filtering schemes such as the one proposed in Ref. [32].

Additionally, even though Eq. (1) was derived by taking into account only virtual particle-hole excitations, real particle-hole excitations will certainly take place during the dynamical evolution. They would lead to oscillations on top of the effective Hamiltonian dynamics with amplitude \( J/U \) and periodicity \( \sim h/U \). Therefore, in order to efficiently average them out one has to work in the strongly correlated regime, i.e., with the condition \( t_{\text{in, out}} \ll U \), though this implies smaller time scales for the dynamical evolution. In typical experiments, work-
ing in a parameter regime where particle-hole excitation effects are negligible requires a superexchange coupling $J/\hbar$ of the order of 1 kHz ($t_s \sim 1$ ms) and thus for a system with approximately 20 lattice sites, it will take about 10 ms to generate entanglement between the atoms at the edges of the cloud.

Another aspect of our procedure is that the long-distance entangled pairs are generated by switching the interactions at specific moments of time. In practice however one always expects switching time uncertainties $\delta t$ and therefore the interval between consecutive steps will not be exactly $t_s$ but $t_s + \delta t$. Such inaccuracies will accumulate and will degrade the quality of the final state exponentially with the number of lattice sites and the number of switches made during the process. Defining the fidelity of a state as $F = |\langle \psi_{t=n t_s} | \psi_{t=0}^{\text{ideal}} \rangle|^2$, where $|\psi_{t=0}^{\text{ideal}}\rangle$ and $|\psi_{t=n t_s}\rangle$ are the ideal and actual states generated after $n$ iterations, one can estimate the degradation of fidelity using Eq. (6)

$$F \sim F_0 (1 - \frac{n(\delta t)^2 N}{4})$$

where $F_0 = |\langle \psi(t=0) | \prod_j |\frac{S_z}{2}, 2j\rangle\rangle|^2$ is the fidelity of the initial state.

D. Entanglement purification

To overcome all the limitations mentioned above one can combine our periodic switching scheme with entanglement purification protocols. Starting from a large ensemble of generated low-fidelity entangled pairs, these protocols distill a smaller sub-ensemble which has sufficiently high fidelity. Entanglement purification can be implemented in a spin-dependent 2D superlattice as follows: after creating an array of $1D$ independent chains along $x$-direction by suppressing tunneling along $y$-direction, one can use our procedure to generate many parallel long-distance entangled pairs within the 1D chains, i.e. an atom at the site $(i, j)$ will be entangled with one at $(i+l, j)$. Then tunneling along the $x$-direction should be inhibited and the following iterative procedures be applied:

1. Lower the intra-well barriers along the $y$-direction of a spin-dependent superlattice, allowing only one of the species to tunnel [33]. This will introduce Ising-type interactions $\sum_j J^y S^z_{i, 2j} S^z_{i, 2j+1}$ between atoms at adjacent sites along $y$-axis and therefore will couple entangled pairs at $(i, 2j) - (i+l, 2j)$ with pairs at $(i, 2j + 1) - (i+l, 2j + 1)$ respectively.

2. Combine the Ising interaction with single-particle rotations, realized with the help of external magnetic fields, to implement the C-Not gate required for the purification schemes described in Ref. [19].

3. Measure the spins at the $(i, 2j)$ and $(i+l, 2j)$ wells. If they turn out to be parallel, keep the correspond-

4. Release the measured atoms and merge the $(i, 2j)$ and $(i, 2j + 1)$ wells into a single one. Repetition of the above protocol will distill from the low-fidelity pairs the ones with higher fidelity.

Let us now briefly discuss the experimental realizability of such purification protocols. To date, one of the main problems is the experimental implementation of step 3 due to the difficulty of measuring individual states at adjacent lattice sites. These atoms are separated by a distance of the order of an optical wavelength and therefore diffraction fundamentally limits individual addressability. One advantage of our scheme is that the atoms in a pair that should be measured are in general separated by many lattice sites, but nevertheless when the measurement is performed on one of the pairs, nearest neighbor atoms are still affected. One possibility to overcome this problem has been proposed recently in Ref. [34] where the use of nonlinear atomic response has been suggested for coherent optical far-field manipulation of quantum systems with resolution of up to a few nanometers. The implementation of the proposals of this kind in the controlled lattice environment may allow proof-of-principle experimental demonstration of quantum purification ideas.

VI. HOMOGENEOUS SWITCH

An interesting question which arises from the dynamics of the periodic switch is what happens with the quantum state if the double wells are no longer decoupled completely, but instead there exists a finite tunneling between them. One expects that in this case the propagation of valence bond states will be suppressed after some period of evolution. To address this question, in this section we consider the case of a homogeneous switch $J_1/J_2 = 1$ (case (3) in our classification), which formally can be considered as a particular case of quench dynamics: we prepare the system in a ground state of one Hamiltonian – a triplet (singlet) product state – and then suddenly change the quantum Hamiltonian to a new one – the isotropic ferromagnetic Heisenberg Hamiltonian $-J$, which determines the subsequent evolution.

In contrast to the periodic switch evolution, whose general characteristics are independent of the singlet or triplet nature of the starting state, the dynamics of the homogeneous switch is strongly affected by the symmetries of the initial state. Consequently, we consider the cases when the initial state is in a triplet (singlet) configuration separately. However, before starting the discussion we first provide a general overview of the dynamics of quantum quenched systems.
A. Quantum quench: general discussion

The time evolution of a quantum state after a quantum quench has recently attracted a lot of theoretical [18, 35, 36] and experimental [25, 37, 38, 39] interest, in part due to the possibility of varying in real time the parameters of the optical lattice. For example, low-dimensional systems prepared in a gapless state and subsequently quenched into an insulator state have been experimentally studied, addressing questions such as relaxation to thermal states and collapse and revival effects. The dynamics of exactly solvable models, e.g. an Ising chain [40, 41, 42], have also been the topic of investigation due to the fact that these systems satisfy many conservation laws which lead to non-trivial equilibration phenomena. Such behavior has been attempted to be explained in terms of a generalized Gibbs ensemble [43]. From the numerical side, recent advances in time-dependent density matrix renormalization group (DMRG) and TEBD methods [20, 21, 44] have allowed to study the quantum dynamics in bosonic and fermionic 1D systems [45, 46, 47]. The numerical simulations seem to support the absence of thermalization, however, these methods are restricted to small and intermediate time scales. The case of the quench from the gapped phase into the critical regime has been studied using conformal field theory by P. Calabrese and J. Cardy [18, 35]. Numerical calculations [47, 48] support their results. The quench dynamics between gapped states can also be attacked using methods of exact solutions [49] and also demonstrate interesting dynamics associated with the absence of thermalization. On the other hand, more conventional approaches based on perturbative methods [50] and diagrammatic expansions [51, 52] inevitably show dynamics associated with thermalization scenario.

In the present work we adopt a numerical approach to deal with the quantum quench dynamics and postpone the analytical treatment for future publications.

B. Initially prepared triplet state

Let us first consider the case of the homogeneous switch dynamics when the initial state is a product of triplet states (Eq. (2)). In order to gain a general understanding of this system, we note that while the initial state has broken rotational and translational symmetries, the Hamiltonian at \( t > 0 \) (ferromagnetic Heisenberg) possesses both of these symmetries. Although its low-energy excitations are dominated by the spin-wave Goldstone modes corresponding to the broken continuous (rotational) symmetry, the quantum dynamics involves a bunch of highly excited modes which know nothing about the spontaneous breakdown of the continuous symmetry. We therefore face a dynamical competition between the initial state with broken symmetries associated with the initial condition on the one hand, and the whole spectrum reflecting both of these symmetries on the other.

As a result of this competition we expect the emergence of a complex magnetic state and the growth of the entanglement entropy.

As we have pointed out, for the correct description of quantum dynamics it is not sufficient to rely on a low-energy effective theory because the details of the spectrum can play a significant role. On the other hand, if we start with a state which involves many excited states, the characteristic features of the dispersion relation of the low-energy modes can be not so important. Also, quantities studied below are invariant under time-inversion symmetry and therefore the dynamics of our problem should have the same common features as that of the antiferromagnetic Heisenberg model. As a result, some common mechanisms should define the generic features of the quantum dynamics of these models. It has been pointed out recently [18, 35] that this generic behavior can be understood in terms of classically moving quasiparticles [18, 36], whose transport correlations are bounded by the light cone (horizon effect). We interpret our results on the basis of these ideas.

1. Entanglement

We first focus on the evolution of the entanglement. The spatially anisotropic and weakly entangled initial state evolves into a highly entangled state with restored translational symmetry. This behavior is signaled by the growth of the entanglement entropy and the rapid decay of the oscillations between even and odd bipartitions.

In Fig. 5 we plot the entanglement entropy of blocks of different sizes in a finite lattice. The plot shows that for short times, after the recovery of translational invariance, the finite-block entanglement entropy exhibits linear growth. A saturation to a value close to the maximal \( S_I = l \) occurs for longer times. This is in agreement with results obtained with the use of conformal field theory [18] that predict a saturation value proportional to \( l \).

The growth of the entanglement limits the applicability of the numerical method (TEBD), as reasonable matrix dimensions (e.g. \( \chi = 1000 \)) are only valid for weakly entangled systems \( (S_I \leq \log_2(\chi) \sim 10) \). Consequently, it is impossible to verify the exact behavior of the entropy for large blocks. However, since in the intermediate time regime the dynamically evolved state in finite lattices does not show significantly lower entanglement compared to an infinite system, to study this regime one can make simulations directly in the infinitely extended periodic system, where the translational symmetry can be exploited. This allows to reduce the computational cost by a factor of \( N \) compared to the finite-lattice simulations [22].

We study the crossover that takes place from the "linear"-growth regime where \( S_I = S_\infty \) \( (S_\infty \) stands for \( S_{even} \), \( S_{odd} \) for even and odd \( l \) respectively), to a saturation towards a constant value. It is probed by the
quantity (see Fig. 5)

$$\Delta S_l = S_\infty - S_l. \quad (16)$$

This crossover is a direct manifestation of the horizon effect. In the case of conformal invariance, where relativistic dispersion relation $\omega_k = v|k|$ is assumed, the distance between entangled atoms is always smaller than $2vt$. The entanglement grows linearly as long as the horizon is smaller than the size of the block. For the open chain considered here, with the block situated at one of the edges, the horizon has to be twice as large as the block length [48]. This allows to define a crossover time $t^* = l/v$ when $S_l[t > t^*]$ becomes a constant [18]. Fig. 5 shows that using the spin-wave velocity of the Heisenberg ferromagnet, $v_s = J\pi/2\hbar$, the crossover indeed takes place around $t^* = l/v_s$. However, comparing results of Fig. 5 with the results of the quantum quench in the $XXZ$-chain [48], we find that the crossover in our case is much slower than in this system. The reason for this is that in a one-dimensional lattice model the sharp crossover is smeared out by lattice effects (which explain why $S_l < S_\infty$ even for $t < l/v_s$) and, more importantly, by the non-linear dispersion relation. Due to the latter, particles moving slower than $v_s$ have to be taken into account, what results in a slower saturation of $S_l(t)$ to a constant value at $t > t^*$.

While long-range effects at the ’horizon’ are determined by the ’fast’ spin waves and the results from conformal field theory are applicable, the slow quasi-particles will be of great importance for understanding the effects related to short-range phenomena.

2. Singlet-triplet population

To study further the dynamical relaxation and the recovery of broken symmetries, we plot in Fig. 6 the singlet-triplet population at adjacent sites $(j, j+1)$. The data are obtained by using an unbiased exact diagonalization technique (Lanczos algorithm [24]) on an open chain with $2N = 22$ sites. After a certain time interval $t_{\text{relax}}$ one expects that the quenched initial values decay into a quasistationary regime, which is destroyed at $t > t_{\text{rec}} = 4N/2v_s$ due to quantum recurrence, when the edges of the expanding light cone begin to interfere [36]. From Fig. 6 we determine that $v_s t_{\text{relax}} \approx 5$; the value $v_s t_{\text{rec}} = 22$ corresponds to a conservative lower bound of the recurrence time. In the quasistationary regime only oscillations around an average value are observed. These oscillations can be associated with the finite bandwidth of quasiparticle energies [35]. We define average values for an arbitrary operator $\hat{O}$ in the quasistationary state.

FIG. 5: The entanglement entropy for the homogeneous switch, $v_s = J\pi/2\hbar$. a) TEBD simulation for $2N = 36$ with open boundary conditions. $S_l$ approaches the line $l$. b) The crossover from linear growth to saturation. Inset: deviation of the finite-block entanglement entropy from the infinite value. The crossover is well characterized by the saturation time defined by the spin-wave velocity, $t^* = l/v_s$.
as follows:

\[ \langle O \rangle_{qs} = \frac{1}{t_{\text{rec}} - t_{\text{relax}}} \int_{t_{\text{relax}}}^{t_{\text{rec}}} dt \langle O(t) \rangle. \]  

Comparing the \( x, y, z \) components of relaxation towards proximate values:

\[ \langle t_{\text{even}}^x \rangle_{qs} = 0.334, \]
\[ \langle t_{\text{odd}}^x \rangle_{qs} = 0.343, \]
\[ \langle t_{\text{even}}^y \rangle_{qs} = 0.267, \]
\[ \langle t_{\text{odd}}^z \rangle_{qs} = 0.272. \]

The relaxation of the singlet-triplet occupation numbers at even and odd bonds towards the same quasistationary values indicates the restoration of the translational symmetry, also suggested by the entropy calculations. The difference between \( t^x \) and \( t^z \) of about 0.06 implies that the rotational symmetry is not completely restored. This difference is stable for various lattice sizes and choices of \( t_{\text{relax}} \) (which by definition allows a certain freedom in its choice). This is a direct indication of missing thermalization in the quasistationary regime. The dynamic state does not fully reflect the symmetries of the Hamiltonian.

3. Structure factor

In Fig. 7 we plot the 'time-dependent' structure factor \( \Delta(q,t) \), which is experimentally accessible by measuring the noise correlations (12). Alongside the persisting peak at \( q = 0 \), the picture shows the formation of a smooth peak at \( q \sim \pi/3a \) for all times \( t > t^* \), which signals the development of an unusual type of magnetic state. We checked that for small lattices (\( 2N = 20 \)) the peak is stable for \( v_\lambda t < 100 \). The height of the peak \( N \Delta(q,t) \) is independent of the lattice size or the type of boundary condition, thus revealing the short-range nature of spatial correlations in the system.

In order to explicitly study the relaxation of the correlation functions and to understand the origin of the incommensurate peak in the noise correlations, we plot in Fig. 8 the real-space correlation function

\[ G^{\pm}(l,t) = \sum_{|i-j|=l} \text{Re}(S_i^+(t)S_j^-(t)) \]  

and the quantity

\[ Q^{\pm}(l,t) = \sum_{|i-j|=l} (-1)^l \text{Re}(S_i^+(t)S_j^-(t)), \]  

which indicates that the translational symmetry is recovered for long-range correlations. The most interesting effect we observe in the correlation functions is the suppression of the ferromagnetic (positive) nearest-neighbor correlations and the development of weak antiferromagnetic (negative) correlations for next-nearest neighbor sites. This is the origin of the incommensurate peak in the noise correlations (Fig. 7). The large-distance properties of the correlation function do not contradict the predictions of conformal field theory [35]. For instance, the correlations are ferromagnetic and change from their initial values only when the 'horizon' of quasiparticle pairs \( l(t) = 2v_\lambda t \) passes, although in this case we find that the horizon is not absolutely sharp. It is important to notice that, although the horizon moves with constant speed, the intensity of the correlations decays fast with larger distances and the correlation length remains finite.

The observed mixed correlations can be interpreted as an implication of energy conservation. At time \( t = 0 \) the whole correlation energy is stored in the short-ranged tripllets; at \( t > 0 \) the action of the evolution operator leads to the formation of longer-distance singlets between spatially separated sites. This singlet component persists for longer times and leads to the appearance of the antiferromagnetic component in the spin-spin correlation function. Therefore the local redistribution of correlation energy, revealed in the partial AF correlation, is one possible explanation for the emergence of mixed correlations.

C. Initially prepared singlet state

In this section we study the case of the homogeneous switch (with dynamical evolution determined by the Heisenberg chain, \( J_1 = J_2 = J > 0 \), Eq. (2)), but instead of starting from a triplet product state, we now start from a singlet product state,

\[ |\psi(t = 0)\rangle = \prod_j |s_{2j,2j+1}\rangle. \]  

FIG. 7: The noise correlations for the infinite lattice, TEBD simulation, \( v_\lambda = J\pi/2\hbar \). A broad peak at \( qa/\pi \sim 1/2 \) appears at \( v_\lambda t \sim 1 \), which shifts towards \( qa/\pi \sim 1/3 \) with the time evolution.
For bosonic systems this state can be experimentally realized by time evolution of the initial triplet product state in the presence of a magnetic field gradient \cite{11}. This initial state also corresponds to the decoupled double-well ground state of the respective fermionic system, though in this case the evolving Hamiltonian is the antiferromagnetic Heisenberg model instead of the ferromagnetic one. However, since the dynamical evolution is independent of the overall sign of the Hamiltonian, the results discussed in this section will also hold for the fermionic system.

Unlike the case of initially prepared triplet state, here the spherical symmetry is not broken, and the populations of the $x, y$ and $z$ components of the triplets are equal. From Fig. 9 we extract that

$$
\begin{align*}
\langle t^{x,y,z}_{\text{even}} \rangle_{qs} & = \langle t^{x,y,z}_{\text{odd}} \rangle_{qs} = 0.125, \\
\langle s^{x,y,z}_{\text{even}} \rangle_{qs} & = \langle s^{x,y,z}_{\text{odd}} \rangle_{qs} = 0.625. 
\end{align*}
$$

These values are a direct consequence of the energy conservation, $\frac{1}{2N} \langle H(t) \rangle = 0.375$. In Fig. 10 we study the spatial correlations. Fig. 10a) shows a rapidly developed broad antiferromagnetic peak in the noise correlations and weak incommensurate peaks at small wave vectors. These are due to large-distance spinon correlations, depicted in Fig. 10b). The fact that the correlations remain negative after the spinon horizon passes (Fig. 10c) can be interpreted as a memory effect of the initial singlet state. Fig. 10c) shows, by investigating the quantity $Q^{+−}(l,t)$ (see Eq. (19)), that the translational symmetry is recovered in the long-range correlation functions, as is the case also for the short-range singlet and triplet correlations.

In general, the prepared singlet product state, due to its initial spherical symmetry, does not exhibit the strong mixing of anti- and ferromagnetic correlations, as the triplet state does. Although the observed spinon correlations are interesting from the theoretical point of view, their weak effect on the noise correlations is barely measurable experimentally. We also note that the spinon correlations may disappear on large time scales which are inaccessible numerically.

VII. CONCLUSION

In this paper we proposed a novel protocol which creates, from a system of two-component atoms initially prepared in an array of triplet (singlet) pairs on neighboring sites, an array of long-distance triplet (singlet) pairs across the lattice. The method allows parallel generation of many entangled pairs, and can have relevant applications for the implementation of quantum purification protocols in optical lattices. We also find that by applying the iterative swapping procedure in an open chain one can engineer a state in which any atom located in the right half of the superlattice is entangled with an atom in
FIG. 10: Correlations for an infinite chain using TEBD simulations, $v_s = J \pi / 2\hbar$. a) The noise correlations for the system prepared in the singlet product state. Besides the strong antiferromagnetic peak there are incommensurate branches for small $q$. b) The real-time correlation function at different moments of time. The correlations converge to an exponentially decaying antiferromagnetic behavior. For larger distances ($l > 6$), a staggered component centered around some finite negative value can be observed. c) The demonstration of how the longer-range correlations remain negative after the passing of the horizon (for even and odd distances).

the left half. This state has maximally separated entangled atoms and persistence of entanglement as large as that of a cluster state, which makes it suitable for being used as a component of a one-way quantum computer [31].

We also studied the evolution of an initial triplet (singlet) product state under a Heisenberg Hamiltonian. Analyzing various observables we showed that while the long-range properties of the evolving state are in agreement with those predicted by conformal field theory, the non-universal short-range properties (e.g. the development of a magnetic state with mixed correlations), are not captured by such theoretical treatments [41] and have to be analyzed more carefully. They might be a manifestation of a special type of thermalization (in the sense of generalized Gibbs ensemble [43]), observed in integrable systems.

The analysis presented in this paper demonstrates that the coherent evolution of an initial state, which itself can be easily prepared – in our case it is just an array of triplet (singlet) states on neighboring sites –, is a feasible way to generate complex magnetic states with cold atoms. The dynamical generation method is not constrained by the difficulty of actual (physical) engineering of exotic Hamiltonians or by the low temperatures required to reach their ground states. On the other hand, without a careful analysis it is difficult to predict a priori the properties of the non-equilibrium state into which the system evolves as a result of coherent quantum dynamics.

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