Efficient generation of many-body singlet states of spin-1 bosons in optical superlattices

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We propose an efficient stepwise adiabatic merging (SAM) method to generate many-body singlet states in antiferromagnetic spin-1 bosons in concatenated optical superlattices with isolated double-well arrays, by adiabatically ramping up the double-well bias. With an appropriate choice of bias sweeping rate and magnetic field, the SAM protocol predicts a fidelity as high as 90% for a 16-body singlet state and even higher fidelities for smaller even-body singlet states. During their evolution, the spin-1 bosons exhibit interesting squeezing dynamics, manifested by an odd-even oscillation of the experimentally observable squeezing parameter. The generated many-body singlet states may find practical applications in precision measurement of magnetic field gradient and in quantum information processing.

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I. INTRODUCTION

A many-body singlet state, theoretically predicted almost two decades ago, is the genuine quantum many-body ground state of an antiferromagnetic spin-1 Bose-Einstein condensate (BEC) [1–5]. It has attracted much attention due to its potential applications in improving gradient magnetometer [6,7], realizing robust quantum states in decoherence-free subspace [8–11], understanding quantum magnetism in frustrated many-spin systems [12–14], and solving no-classical-solution problems in quantum information processing, such as N strangers, secret sharing, and liar detection [15]. Nevertheless, due to the extremely strict requirement of an ultralow magnetic field in the order of microgauss, the many-body singlet state has not yet been realized in experiments.

Much effort has been devoted experimentally to achieving an extremely weak magnetic field environment, which is a must to realize the quantum ground state of an antiferromagnetic spin-1 23Na condensate. A remarkable advance has been made by Hirano’s group, who suppressed their magnetic field within the range of 10 μG, using an active compensation technique in an expensive permalloy-metal-shielded room [6]. However, even in such an ultralow magnetic field, it is not clear whether a robust antiferromagnetic ground state, in the form of the quantum many-body singlet state, can be reached in realistic experimental time scales.

Inspired by the merging of a few spin-1 bosons in a double well [16–19], we propose in this work a stepwise adiabatic merging (SAM) protocol to generate the quantum many-body singlet state, by propagating adiabatically the antiferromagnetic spin-1 bosons in concatenated optical superlattices from an experimentally accessible initial state to the final (ground) quantum many-body singlet state. Briefly, we start with a Mott insulator state of spin-1 bosons with single occupancy for each lattice site, with all the atoms optically pumped to the polar (i.e., |F = 1, m_F = 0⟩) state, then slowly merge the nearest two lattice sites adiabatically along the x direction, and generate many two-body spin singlet states. Next, we merge again the adjacent two sites along the y and z directions to obtain many eight-body singlet states. By further merging the next concatenation level optical lattice with longer wavelength, we obtain many 64-body singlet states. For L-level concatenation optical superlattices, the final singlet states are in principle 8^L-body. The limitation on this SAM protocol is mainly the total evolution time, which is limited by the boson’s lifetime. Such a limitation can be alleviated by optimizing the protocol in an appropriate magnetic field. While in numerical simulations, we are also constrained by the computational power to a system size of 16 bosons. In this method, the final probability of the 16-body singlet state generated through the SAM protocol is above 90% in our numerical simulations under current experimental conditions. The major advantage of our protocol is that it does not require an ultralow magnetic field, which is the limiting factor that prevents a direct realization of the many-body singlet state.

The paper is organized as follows. In Sec. II, we describe the system of antiferromagnetic spin-1 atoms trapped in a double-well unit and the SAM protocol to generate many-body singlet states. In Sec. III, we discuss in detail three key ingredients of the SAM protocol: the bias sweeping range, applied magnetic field, and evolution of the separated SAM steps. In Sec. IV, we present a complete dynamical process to generate a 16-body singlet state with a fidelity as high as 90%. The experimental observable, the generalized spin-squeezing parameter, is also discussed in this section. The conclusions are given in Sec. V. More details about the Hamiltonian, the numerical calculation, the oscillation of the fidelity, and the robustness of the SAM protocol are discussed in the appendixes.

II. HAMILTONIAN AND SAM PROTOCOL

We consider an ultracold dilute gas of bosonic atoms with hyperfine spin F = 1 trapped in a concatenated optical superlattice with isolated double wells in an external magnetic field along the z direction. Such a system is described exactly by the standard Bose-Hubbard model with spin degrees of freedom [18,20,21]. Due to the conservation of the total particle number and total magnetic quantum number (set as zero here), the linear Zeeman term does not affect the dynamics of the system, thus only the quadratic Zeeman effect is taken
The Hamiltonian is
\[
H = -J \sum_{\sigma=\pm 1,0} (\hat{L}_\sigma^\dagger \hat{N}_\sigma + \hat{N}_\sigma \hat{L}_\sigma^\dagger) + \frac{U_0}{2} \sum_{i=L,R} \hat{N}_i(\hat{N}_i - 1) \\
+ \frac{U_2}{2} \sum_{i=L,R} (\hat{S}_i^2 - 2\hat{N}_i) + \epsilon(\hat{N}_L - \hat{N}_R) + H_Z. \tag{1}
\]

The first term describes the tunneling between wells in a double-well unit where \( J = \int d^3r \psi^\dagger_\sigma(r)(-\hbar^2\nabla^2/2M) + V(r)\psi_\sigma(r) \) depicts the tunneling amplitude with \( \psi_{L,R}(r) \) the wave function in (left) right well, \( M \) the atom mass, and \( V(r) \) the effective potential for the double well. The creation and annihilation operators \( \hat{L}_\sigma \) and \( \hat{R}_\sigma \) for the hyperfine spin state \( \sigma \in \{-1,0,1\} \) in the left (right) well obey the canonical bosonic commutation relations. The intrawell density interaction is described by the repulsive \( U_{0,2} \) and \( U_2 \) terms, respectively, the \( s\)-wave scattering length of two colliding bosons with total angular momenta 0 and 2 \([1-3]\). The intrawell antiferromagnetic spin exchange interaction is described by the \( U_2 > 0 \) term, where \( \hat{S}_\sigma = \sum_{\sigma’} \hat{L}_\sigma^\dagger \hat{F}_{\sigma\sigma’} \hat{L}_{\sigma’} \). The total spin in the double well is generated. Continuously adiabatically ramping up along the direction \( \sigma \) for the intrawell spin exchange interaction.

**III. THREE KEY INGREDIENTS**

Before we present the complete evolution of the spin-1 bosons under the SAM protocol, let us discuss the three key ingredients separately. First, we need to determine the sweeping range of the double-well bias for each SAM step. Such a range is determined by exploring the dependence of \( N_R \), the occupation number of the lower well which we refer as the “right” well hereafter, on the double-well bias \( \epsilon \) for the ground state of the Hamiltonian in Eq. \( (A1) \). The results are shown in Fig. 2 for the merging of 2–16 atoms. It can be seen that \( N_R \) increases in steps of one as the bias increases.

Such a single-atom tunneling is due to the strong intrawell repulsion, \( U_0 > J \). This kind of behavior has been investigated in theory \([28-30]\) and confirmed in experiment \([16]\). The atom number \( N_F \) eventually reaches its maximum at a large bias \( \epsilon_f \), thus the range is \([0, \epsilon_f]\). The merging of larger number of atoms requires a larger bias range, roughly in a linearly increasing form. This in fact manifests the linear relation between the chemical potential and the number of atoms in a double well, \( \epsilon_f = \left(U_0/2\right)N(N-1) - E_b \) with \( E_b \approx (U_0/4)N(N-1) \) being the energy of the system in a balanced double well \( \epsilon = 0 \).

Second, we determine the range of the magnetic field, in which the ground state is close to the expected initial state of each SAM step. According to the protocol, the ideal initial state \( |\psi_F\rangle \) is the product state of the left and right well with...
parameters are the same as in Fig. 1 except that here $q = 0$. In the SAM protocol, $\varepsilon \geq 0$ is required.

We plot the probability $P_0$ in Fig. 3. For $N = 2$ atoms, the probability $P_0$ increases as $q$ increases in the low bias $|\varepsilon|$ region. Thus, the expected initial state $\psi_E$ can be prepared in a large magnetic field at zero (low) bias. For $N > 2$ and even number of atoms, the probability $P_0$ is high around the central region, i.e., low bias ($\varepsilon$) and low quadratic Zeeman energy ($|q|$) region. In order to generate a final many-body singlet state with a probability higher than 90% with the SAM protocol, we are limited to choosing a set of $\varepsilon$ and $q$ within the enclosed region marked by the white dashed line (where $P_0 > 90\%$).

As shown in the figure, the largest quadratic Zeeman energy on the white dashed line is $q/U_2 = 0.64$, 0.34, and 0.054 in the Figs. 3(b), 3(c) and 3(d), respectively. The enclosed region becomes smaller and smaller as $N$ increases, indicating that the generation of larger many-body singlet states becomes more and more challenging [31]. This is the main reason why the many-body singlet state has not been observed experimentally though it has been predicted theoretically for almost two decades [2,4,5].

Third, we investigate the performance of the separated SAM steps for a fixed even number of atoms in a double-well unit, by assuming an ideal initial state $|\psi_E\rangle$ [32]. During the evolution, we adiabatically ramp up the bias at a constant rate from zero to a final value $\varepsilon_f$. The evolution of the system is monitored by two observables, the number of atoms in the right well $N_R$ and the fidelity $F = |\langle \Psi(t) | \Psi_S \rangle |^2$ with $|\Psi_S\rangle$ being the state vector at time $t$ and $|\Psi_S\rangle = |N, S = 0, M_S = 0\rangle$ the targeted $N$-body singlet state.

We illustrate the evolution of the generation of the many-body singlet states according to the SAM protocol in Fig. 4 for atom numbers $N = 2, 4, 8,$ and 16 at four chosen quadratic Zeeman energies. The fidelity increases sharply from zero to an almost constant at time $t_c$, which coincides with the time when the right-well atom number $N_R$ approaches the total number of atoms $N$ [see Fig. 4(c)]. The highest fidelity for each $N$ is above 90% among the four selected quadratic Zeeman energies within an appropriate evolution time. From Fig. 4, we also observe that the fidelity at the end of evolution exhibits oscillations with increasing quadratic Zeeman energy, indicating the existence of an optimal magnetic field in a realistic experimental situation [27].

IV. EFFICIENT GENERATION OF SINGLET STATES

Finally, to present a complete view, we carry out a continuous evolution process to efficiently generate a 16-body singlet...
state from a singly occupied polar state in a concatenated optical superlattice, according to the SAM protocol shown in Fig. 1. The sweeping rate of the bias is a constant during each step. However, the sweeping rate is adjusted for different steps [see the lines in Fig. 1(d)] in order to limit the total evolution time in an experimentally accessible regime. The total number of atoms of the generated singlet state is in principle doubled as the product of the final state in the lower well and its copy. Such an operation is nonunitary so that the total number of atoms \(N\) as well as the atoms in the lower well \(N_R\) in fact decrease at this connecting point, as shown in Fig. 1(e). However, the product state at the beginning of each SAM protocol is important to reduce the computational basis from an exponential increasing \(3^N\) to a much slower way, see Table I in Appendix C.

The fidelities of the many-body singlet state are presented in Fig. 1(f). Clearly, the SAM protocol is efficient to produce the many-body singlet states with high fidelity. As a trend, the larger the size of the many-body singlet state, the lower the final fidelity. Such a decline in fidelity is caused by two sources, the nonadiabaticity during the evolution and the atom loss between two adjacent SAM steps. The nonadiabaticity-caused fidelity declination may be prevented by sweeping the bias with a slower rate or by employing nonlinear sweeping function, such as the shortcut to adiabatic passage [33]. The atom-loss-caused fidelity dropping can be improved by utilizing the experimental technique of postselection, i.e., we only take into account the results having the number of atoms in the lower well and its copy. Such an operation is nonunitary so that the total number of atoms \(N\) as well as the atoms in the lower well \(N_R\) in fact decrease at this connecting point, as shown in Fig. 1(e). However, the product state at the beginning of each SAM protocol is important to reduce the computational basis from an exponential increasing \(3^N\) to a much slower way, see Table I in Appendix C.

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APPENDIX A: HAMILTONIAN OF THE SYSTEM

We consider a dilute gas of bosonic atoms with hyperfine spin $F = 1$ trapped in a concatenated optical lattice with isolated double wells in an external magnetic field along the $z$ direction. This system conserves the total particle number $N$ and total magnetic quantum number (set as $M = 0$ here), thus only the quadratic Zeeman effect is taken into account. The Hamiltonian of the system, Eq. (1) in the main text, is expanded as $[18,20,21]$

$$H = \frac{U_0}{2} [\hat{N}_L (\hat{N}_L - 1) + \hat{N}_R (\hat{N}_R - 1)] - J (\hat{a}^\dagger_{L-1} \hat{a}_{R-1} + \hat{a}^\dagger_{R-1} \hat{a}_{L-1} + \hat{a}^\dagger_{L1} \hat{a}_{R1} + \hat{a}^\dagger_{R1} \hat{a}_{L1})$$

$$+ \epsilon (\hat{N}_L - \hat{N}_R) + \frac{U_2}{2} (|\hat{S}|^2 - 2\hat{N}_L) + \frac{U_2}{2} (\hat{S}_R^2 - 2\hat{N}_R)$$

$$+ q (\hat{N}_{L1} + \hat{N}_{L-1} + \hat{N}_{R1} + \hat{N}_{R-1}).$$ \hspace{1cm} (A1)

The coefficients $U_0, J, U_2, q$ have been described in the main text. $\hat{N}_i = \hat{a}^\dagger_i \hat{a}_i + 1$, $\hat{a}^\dagger_0 \hat{a}_0$, and $\hat{a}^\dagger_{-1} \hat{a}_{-1}$ is the atom number operator in the $i$th $(i = L, R)$ well. The components of the spin-1 vector $\mathbf{S}$ are written as creation and annihilation operators,

$$\hat{S}_x = \frac{1}{\sqrt{2}} (\hat{a}^\dagger_1 \hat{a}_0 - \hat{a}^\dagger_0 \hat{a}_1 + \hat{a}^\dagger_0 \hat{a}_{-1} + \hat{a}^\dagger_{-1} \hat{a}_0),$$

$$\hat{S}_y = \frac{i}{\sqrt{2}} (\hat{a}^\dagger_1 \hat{a}_0 + \hat{a}^\dagger_0 \hat{a}_1 - \hat{a}^\dagger_0 \hat{a}_{-1} - \hat{a}^\dagger_{-1} \hat{a}_0),$$

$$\hat{S}_z = (\hat{a}^\dagger_0 \hat{a}_1 - \hat{a}^\dagger_1 \hat{a}_0).$$ \hspace{1cm} (A2)

Based on these equations, the $U_2$ terms in Eq. (A1) become

$$\frac{U_2}{2} (|\hat{S}|^2 - 2\hat{N}_L) = \frac{U_2}{2} [\hat{N}_{i1} (\hat{N}_{i1} - 1) + \hat{N}_{i-1} (\hat{N}_{i-1} - 1)]$$

$$+ 2\hat{N}_{i1} \hat{N}_{i0} + 2\hat{N}_{i0} \hat{N}_{i-1} - 2\hat{N}_{i1} \hat{N}_{i-1}$$

$$+ 2\hat{a}^\dagger_0 \hat{a}^\dagger_1 \hat{a}_1 \hat{a}_{-1} + 2\hat{a}^\dagger_{-1} \hat{a}^\dagger_{-1} \hat{a}_0 \hat{a}_1],$$ \hspace{1cm} (A3)

where $\hat{a}^\dagger_\sigma (\hat{a}_\sigma)$ is the creation (annihilation) operator of the hyperfine state with $\sigma \in \{-1,0,1\}$.

APPENDIX B: CONSTRUCTION OF MANY-BODY SINGLET STATES

The many-body spin singlet state, $|N,S = 0, M_S = 0\rangle$, consisted of $N$ particles with total angular momentum quantum number $S = 0$. For a two-body singlet state, the $|2,S = 0, M_S = 0\rangle$ can be theoretically produced by acting the singlet pair operator $\hat{A}^\dagger = [(\hat{a}^\dagger_0)^2 - 2\hat{a}^\dagger_0 \hat{a}^\dagger_{-1}] / \sqrt{3}$ on the vacuum state $\langle \text{vac} \rangle$ with the following normalization:

$$|2,S = 0, M_S = 0\rangle = \sqrt{\frac{1}{3}} |0,2,0\rangle - \sqrt{\frac{2}{3}} |1,0,1\rangle.$$

where the state $|k, N - 2k, k\rangle$ for $k = 0, 1$ denotes the basis of Fock states. For even $N$ atoms, the singlet state $|N,S = 0, M_S = 0\rangle$ is constructed by acting the singlet pair operator, consequently $|2,4,5\rangle, |N,S = 0, M_S = 0\rangle = (\hat{A}^\dagger)^n |\text{vac}\rangle$.

APPENDIX C: DIAGONALIZATION OF THE HAMILTONIAN

We work in the computational basis of the Fock space in an isolated double-well unit, $|N_{L1}, N_{L0}, N_{R1}, N_{R0}, N_{R-1}\rangle$. We set the parameters $U_2 = 1$, and $U_0/U_2 = c_0/c_2 \approx 27.8$ for $^{23}$Na spin-1 Bose-Einstein condensates and $J/U_2 = U_0/40 \approx 0.694$ throughout the paper [17,38,39]. The number of basis states $K$ of $N$ atoms in a double well increases roughly in an exponential form, as shown in Table 1.

In the main text, Fig. 2 was obtained by searching for the ground state via diagonalizing the Hamiltonian with zero quadratic Zeeman energy for different potential biases $\epsilon$. Then we calculated the expectation value of the atom number in the right well $N_R = \langle \hat{N}_R \rangle$. Similarly, the probability $P_0$ in Fig. 3 was obtained by calculating the overlap of the ideal many-body singlet product state (the polar product state for $N = 2$) with the found ground state at different quadratic Zeeman energies $q$ and different potential biases $\epsilon$.

For the SAM protocol shown in Fig. 1, the minimum gaps $\Delta$ between the instantaneous first excited state and the ground state are $0.07 U_2, 0.05 U_2, 0.13 U_2$, and $0.27 U_2$ for the SAM steps during the generation of the two-, four-, eight-, and 16-body singlet states, respectively. Multiplied by the evolution time $T$ of each SAM step, we find $\Delta T \geq 1$. This relation roughly satisfies the adiabatic condition.

APPENDIX D: OSCILLATIONS OF FIDELITY

We observe in Fig. 4 some signatures of oscillatory behavior of the fidelity for the four chosen values of the quadratic Zeeman energy. A more systematic investigation of the fidelity dependence on the total evolution time and the quadratic Zeeman energy are presented in Figs. 5 and 6 for $N = 2$ and $N = 4$ atoms, respectively. The fidelities are the final value at the end of the evolution with the given quadratic Zeeman energy. The bias sweeps linearly from zero to $\epsilon_f = 20U_2$ for $N = 2$ atoms and to $60U_2$ for $N = 4$ atoms.

| Table I. Number of basis states $K$ increases roughly exponentially with the number of atoms $N$ in a double-well unit system. |
|---|---|---|---|---|---|---|
| $N$ | 2 | 4 | 8 | 16 | 32 |
| $K$ | 7 | 26 | 155 | 1365 | 15657 |

Note: $K$ increases roughly exponentially with the number of atoms $N$ in a double-well unit system.
From Fig. 5 we observe an oscillation with the quadratic Zeeman energy for a fixed evolution time. As shown in the figure, the fidelity is not very sensitive to the change of the total evolution time. While for the quadratic Zeeman energy, there exists a pretty large optimal region around 0.25 where the fidelity is high.

In Fig. 6 there is a high-fidelity region with weak dependence on the total evolution time near zero quadratic Zeeman energy. As the quadratic Zeeman energy increases, the fidelity shows many oscillations and there are several high-fidelity bands. These results indicate that one needs to set wisely in an experiment the quadratic Zeeman energy and the evolution time, in order to reach a high fidelity of many-body singlet state.

APPENDIX E: ROBUSTNESS OF THE SAM PROTOCOL

In experiments, the magnetic field may fluctuate from shot to shot. To test the robustness of the proposed SAM protocol, we assume uniformly distributed random magnetic fields around its averages, 141.4 mG ($q/U_2 \approx 0.1108$ for $^{23}$Na atoms with $U_2 = 50$ Hz) for the two-body singlet state and 35.4 mG ($q/U_2 \approx 0.0069$) for the higher-body singlet state. The magnetic field fluctuation is within 1 mG, which is easily realized with current experimental techniques. The results for 100 realizations are shown in Fig. 7 and the averages and typical error bars are shown in Fig. 8. Clearly, the final fidelities of the 16-body singlet state only fluctuate in a small range, indicating the robustness of the SAM protocol.
[27] See the appendixes for more detailed discussions on the Hamiltonian, numerical procedure, fidelity oscillation, and effect of magnetic field fluctuations.
[31] For example, the quadratic Zeeman energy $q/U_2 < 0.36$ is required to satisfy $P_0 > 90\%$ at $\epsilon = 0$ in Fig. 3(c), but it drops to $q/U_2 < 0.054$ in Fig. 3(d).
[32] For an even $N$ atom system, the initial state is set as a product state of two singlet states with $N/2$ atoms each. While for $N = 2$ atoms, the initial state is a product state of two polar states with a single atom in each well.