Observation of antiferromagnetic correlations in an ultracold SU(N) Hubbard model

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Mott insulators are paradigmatic examples of strongly correlated physics from which many phases of quantum matter with hard-to-explain properties emerge. Extending the typical SU(2) spin symmetry of Mott insulators to SU(N) is predicted to produce exotic quantum magnetism at low temperatures. In this work, we experimentally observe nearest-neighbour spin correlations in a SU(6) Hubbard model realized by ytterbium atoms in optical lattices. We study one-dimensional, two-dimensional square and three-dimensional cubic lattice geometries. The measured SU(6) spin correlations are enhanced compared with the SU(2) correlations, owing to strong Pomeranchuk cooling. The experimental data for a one-dimensional lattice agree qualitatively with our theoretical calculations, with an error of at most 30%, without any fitting parameters. Detailed comparison between theory and experiment allows us to infer the temperature to be the lowest achieved for a cold-atom Fermi–Hubbard model. For three-dimensional lattices, the experiments reach entropies below the regime where our calculations converge, highlighting the importance of these experiments as quantum simulations.

A recurring question regarding many-body quantum systems is how the competition between the kinetic and interaction energies determines the ground-state quantum phases. Quantum fluctuations play an essential role in determining the ground-state spin structure, which may differ drastically from the mean-field prediction. The SU(2) Hubbard model has long been a prototypical system to study these effects, and Hubbard models with an enlarged SU(N) symmetry have attracted great interest.

The study of SU(N) quantum magnetism historically originated from the mathematical technique of large-N expansions1–4. More recently, understanding N>/2 systems has attracted broader interest owing to the expectation that such systems will display a wide array of exotic physics5–11. Although N can be large, quantum fluctuations remain important since SU(N) symmetry prevents spins from becoming classical12,13.

Although theoretical models with SU(N) symmetry have also been discussed in connection with real physical systems such as transition-metal metal oxides14,15 and graphene’s SU(4) spin-valley symmetry16,17, the introduction of the symmetry is just a rough approximation. In contrast, an intrinsic SU(N) nuclear spin symmetry18,19 is realized in fermionic isotopes of alkaline earth metal-like atoms (AEAs), providing unique opportunities for quantum simulation experiments of the SU(N) Fermi–Hubbard model (FHM)19–24. The SU(N=2†+1) FHM can be implemented by loading an AEA with a nuclear spin I in an optical lattice. This model is given by the Hamiltonian

$$H = -t \sum_{\langle i,j \rangle} c_{i \sigma}^\dagger c_{j \sigma} + \frac{U}{2} \sum_{\langle i \neq j \rangle} n_{\sigma}(i) n_{\sigma}(j) - \mu \sum_{i, \sigma} n_{\sigma}(i),$$

where $c_{\sigma}$ ($c_{\sigma}^\dagger$) denotes the fermionic annihilation (creation) operator for site $i$, $n_{\sigma}(i) = c_{\sigma}^\dagger c_{\sigma}$ is the number operator and $\mu$ is the chemical potential that controls the density. The flavour index $\sigma$ labels the projection quantum number of the nuclear spin $m_f$. Here we employ $^{173}$Yb, and $m_f = -5/2, -3/2, ..., +5/2$. The tunnelling amplitude $t$ and the on-site interaction $U$ do not depend on $\sigma$, giving rise to the SU(N) symmetry.

An important characterization of strongly correlated states is provided by their spin correlation functions. For the SU(2) Hubbard model, antiferromagnetic (AFM) correlations were first observed in dimerized lattices29, in un-dimerized three-dimensional (3D) lattices using Bragg spectroscopy26 and in one-dimensional (1D) and two-dimensional (2D) lattices using quantum gas microscopy27,28. However, correlations in a uniform SU(N) Hubbard model have not been observed previously. Although observing long-ranged correlations would be essential to characterize phases of matter and their phase transitions, nearest-neighbour spin correlations are already of great interest. In many models, the most rapid change of nearest-neighbour correlations with temperature can be a proxy for the critical temperature, and short-ranged correlations are a key ingredient in pair formation in cuprate and iron–pnictide superconductors, where short-ranged magnetic correlations appear to be essential for the pairing29–31. In this work, we observe the nearest-neighbour AFM spin correlations in an SU(6) $^{173}$Yb Fermi gas loaded in 1D, 2D and 3D optical lattices and measure them as a function of the initial entropy in a harmonic trap. These experimental results are compared with theoretical calculations with no fitting parameters.

**Experimental setup**

Figure 1a depicts our physical system. The SU(6) Fermi gas of $^{173}$Yb with atom number $N_{\text{ptcl}}=2.4(1)\times10^4$ is adiabatically loaded into 1D chain, 2D square and 3D cubic lattices that are constructed by a primary optical lattice operating at 532 nm (Methods). The 1D chain and 2D square lattices are created by introducing strong...
tunnelling anisotropy into the cubic lattice. The inter-lattice tunnelling is less than 5% of the intra-lattice tunnelling and is much smaller than the other energy scales in the system. In our previous work\(^1\) we measured the spin correlation of SU(4) fermions loaded into a double-well system in which the nearest-neighbour correlation is artificially enhanced by strong dimerization. However, in the present work, the SU(6) fermions are loaded into uniform lattices in 1D, 2D and 3D in which there is no trivial enhancement of spin correlations due to dimerization.

One can utilize the technique of singlet–triplet oscillations (STO)\(^\text{3,5,8}\) in an optical superlattice to measure the nearest-neighbour correlations, including for SU(N) Fermi gases\(^5\). The principle of the STO measurement is illustrated in Fig. 1b. Tunnelling is frozen except between pairs of adjacent lattice sites along the measurement axis, which are merged into single sites of a detection lattice with twice the spacing. Here, we utilize the fact that s-wave photoassociation (PA) only associates pairs of atoms with a spatially symmetric wavefunction and thus is only sensitive to spin antisymmetric states in each detection site since the total wavefunction is antisymmetric. Associated molecules quickly escape from the trap, resulting in atom loss. Application of a spin-dependent potential gradient before the merging process drives oscillations of spin symmetry, enabling us to also detect spin symmetric states. These are not to be confused with SU(N) singlets and triplets, which are N-body entangled states\(^5\). The STO measurement is valid only if the contribution from multiple occupancies can be neglected. For this reason, we set the central density to unit filling and the interaction strength is \(U/t=15.3(5)\). The error bars represent the standard deviation for the six independent measurements. STO measurement with OSG spin separation. Top: Absorption image of the OSG.
as an alternative measure. As long as the SU(N) symmetry holds, A is proportional to the spin distribution of the SU(N) spin correlation function $C_{NN}$ (ref. 13) (Methods) given by

$$C_{NN} = \sum_{\sigma \neq \tau} \langle n_{\sigma}(i) n_{\sigma}(i+1) \rangle - \langle n_{\sigma}(i) n_{\tau}(i+1) \rangle,$$

where $n_{\sigma}(i+1)$ is a shorthand we use throughout for number operators at a nearest neighbour of $i$. In the trap, $A$ will be drastically reduced compared with the uniform unit filled case because of the low density at the edge of the sample, and incorporating the effect of harmonic confinement is important to compare calculations of $A$ with experiments. Note that the singlet and triplet fractions can be determined if we know both $I$ and $A$.

Figure 1c shows a typical STO signal measured in a 1D chain lattice. To create the spin–dependent potential gradient, we utilize linearly polarized laser light close to the $^1S_0 \rightarrow ^3P_0$ resonant frequency (Methods). As a result, STOs are driven for the spin pairs with different $|m_I|$ values (1/2, 3/2, and 5/2), resulting in three different STO frequencies. The ratio of these frequencies $\omega_{1/2} : \omega_{3/2} : \omega_{5/2} = 1 : 2 : 3$ is determined by the Clebsch–Gordan coefficients and does not depend on detuning (Methods). We analyse the STO signal, assuming the SU(N) symmetry, namely that all spin combinations contribute equally to correlations. Along the chain axis, we obtain a singlet–triplet imbalance of $I = 0.674 \pm 0.052$, indicating the large AFM correlation ($C_{SU} < 0$). On the other hand, correlations between chains are zero within the error bar ($I = 0.01 \pm 0.01$) as expected from the negligible inter-chain tunnelling.

To verify the expected SU(6) symmetry, we observe the time evolution of each nuclear spin component during STOs. After the standard STO process (driving STO, merging double wells and applying PA), lattice potentials are ramped down adiabatically in 6 ms to suppress momentum spread. Then, we turn off the optical trap, followed by the application of the optical Stern–Gerlach (OSG) beam for 0.2 ms. The OSG light source is identical to that used for the gradient beam for driving STO but with nearly three times higher intensity. Therefore, the OSG beam is $x$ polarized and distinguishes only spin components with different $|m_I|$. Figure 1d shows analysis of the spin distribution. The behaviour is well reproduced by the two-frequency model (Methods), indicating that the STO scheme is working as designed. The fit to oscillations of the $|m_I|=1/2$ cloud seems slightly worse than the others. This is due to the stronger deformation of the cloud and possibly spin flips caused by the photon scattering from the OSG laser. We confirm that the deviation of each spin population from the balanced mixture is about 3% and this does not affect the following results.

**Results**

Antiferromagnetic nearest-neighbour spin correlations. Figure 2a,b shows the nearest-neighbour correlations for the 1D and

![Fig. 2](image-url)
3D lattices as a function of entropy per particle, with a dramatic enhancement of SU(6) spin correlations compared with the SU(2) correlations in the 1D system. The total entropy $S$ is inferred from a time-of-flight measurement of the weakly interacting gas before lattice loading. The on-site interaction is fixed to $U/t = 15.3$ for all lattice configurations, which is determined from the band calculation with measured lattice depths. In this strongly interacting regime, an important scale is the maximum spin entropy per particle for a singly occupied site, given by $S_{\text{spin}}^{(N)} = k_B \ln N$, where $k_B$ denotes the Boltzmann constant. Naïvely, ignoring the spatial inhomogeneity of the trap, a sample with $S/N_{\text{ptcl}} < S_{\text{spin}}^{(N)}$ is expected to reach the temperature regime where the spin correlations emerge. For SU(6), $S_{\text{spin}}^{(6)} = 1.79k_B$, while for SU(2), $S_{\text{spin}}^{(2)} = 0.69k_B$, and $N = 6$ systems are therefore expected to show remarkably enhanced correlations, which is interpreted as the enhancement of the Pomeranchuk effect due to large spin enhancement. Our microscopic theory confirms this simple picture, and the observed data show reasonable agreement with theoretical predictions obtained by exact diagonalization (ED) for 1D and by determinantal quantum Monte Carlo (DQMC) for 3D, without any fitting parameters.

Here, we suggest a possible origin of the small deviation observed between the theory and experiment. Given the extensive tests we have done on our codes and experiments, we consider an actual error in the calculations or the experiments unlikely. The remaining possibility is the fundamental differences between the model being simulated and the atomic system being measured. On the computational side, we have carefully investigated Trotter errors, finite-size effects and the use of the local density approximation (LDA) (Methods). The calculations assume that the loading is adiabatic, while non-adiabatic loading of the atoms to the lattice may play some role in the experiments. For the 1D SU(6) case, the correlations measured in the low-entropy region are smaller than the theoretical curve by ~30%, and it is plausible that the main source of the discrepancy is the non-adiabaticity of the lattice loading. We estimate the amount of heating to be $0.2k_B$ around the lowest temperature (Methods). For the higher-entropy region in the 1D SU (6) case, on the other hand, the measured correlations are larger than the theoretical predictions. Although experiments start with a weakly interacting gas, it is possible that some of the initial correlations are frozen during lattice loading, which could be a source of the small remaining discrepancies between the experimental results and theory.

Figure 2c–e shows theoretically calculated trap profiles of atom number, entropy and nearest-neighbour spin correlations per site for a 1D system. A rigid Mott plateau is well developed at $k_B T/t \approx 0.5$, and spin correlation develops rapidly for lower temperature. Estimation of the temperature obtained in our experiment is discussed in the next section.

### Extracting temperature in an optical lattice by theory–experiment comparison

The present experiments cannot directly measure the temperature at the very low entropies studied here. However, for the 1D systems, the temperature can be inferred by comparing experiment and theory. In 1D, the lowest temperature achieved in the experiments is $k_B T/t = 0.096 \pm 0.054 \pm 0.030$, obtained from the singlet-triplet imbalance $I$ measured experimentally at $S/N_{\text{ptcl}}/k_B = 1.45 \pm 0.05$ (Extended Data Fig. 1). The first error is an estimate of the finite-size error given by the difference between the finite-size extrapolation to the thermodynamic limit and the eight-site result. The second error comes from the experimental uncertainty on the correlations. This is lower than the state-of-the-art temperatures reported in cold-atom FHM systems. Estimates based on $A$ rather than $I$ are similar (Methods). The agreement between theory and experiment in 1D suggests the reliability of the experiment in higher dimensions where numerics fail and quantum simulation via experiment is crucial.

For comparison, at the same entropy, the SU(2) system is at $k_B T/t = 1.008 \pm 0.073 \pm 0.001$, or to obtain the same singlet–triplet imbalance $I$ measured experimentally at $S/N_{\text{ptcl}}/k_B = 0.499 \pm 0.136 \pm 0.120$. Since the state-of-the-art averaged entropy per particle for SU(2) experiments with alkali atoms is around $k_B$, this suggests an experimental advantage for SU(N) systems in obtaining highly correlated states in optical lattices.

### Dependence on lattice dimensionality

In addition to the dependence on $N$, the correlations depend drastically on dimensionality, with the 1D case exhibiting the largest correlations as shown in Fig. 3a,b. This behaviour is similar to previous studies in an SU(2) system and can be understood at sufficiently high temperatures.

In this regime, correlations depend only on temperature and not dimensionality. This intuitive result can be proved with a high-temperature expansion and decrease with increasing temperature. Additionally, decreasing dimension decreases the bandwidth and thus, at fixed entropy, decreases the temperature (Fig. 3b). Together, these imply that correlations decrease as the dimensionality is increased. The situation at lower temperatures is expected to be more complicated, but the numerics indicate that this simple conclusion remains true.
Constructions simple arguments for the low-temperature regime remains an interesting challenge.

Figure 3a shows the singlet–triplet imbalance measured through 1D–2D and 2D–3D crossovers with the same initial condition. We measure the correlations along the z-axis and change the ratio of $t_\perp$ to the tunnelling $t_z$ of the initially weak link. At both the maximum and minimum $t_\perp/t_z$ and at the intermediate point $t_\perp/t_z = 1$, we set $U/t_z = 15.3$. The lattice geometry is changed smoothly between the above three points (see also Methods). We find that spin correlations decrease monotonically as the lattice is deformed from 1D to 2D. For the 2D–3D crossover, the difference is smaller but the trends of decreasing correlations with increasing dimensionality are still visible. The correlation drops quickly for $t_\perp/t_z < 1$ and becomes undetectable, as expected.

Numerical calculations show a similar trend. Although DQMC has difficulty in obtaining reliable results for 3D systems at the low temperatures where remarkable correlations develop for $U/t_z = 15.3$ and $N = 6$, it can calculate the properties of 3D systems for $U/t_z = 8$ and $N = 3$ to low temperature where remarkable correlations develop. Because we are considering a smaller $N$, we calculate ED results without using the basis state truncation for 1D $L$-site chains with $L = 4–7$. Figure 3b presents the computed entropy per particle and the spin correlations. Although these are not directly the conditions in the experiments, they do show the same trend of correlations decreasing with increasing dimension.

DQMC results for $N = 6$ are only presented at temperatures above $T/t_z = 1$, owing to a strong sign problem below this temperature, as well as the onset of non-ergodicities in the Monte Carlo sampling in this region. The sign problem is particularly strong in the metallic region, where large errors in the observables appear for several values of the chemical potential. Reference 13 provides more details on how the sign problem depends on $U/t_z$ and $\mu/t_z$.

**Discussion**

We find that the measured nearest-neighbour AFM correlations agree broadly with the theory with no fitting parameters for all temperatures in 1D, and at temperatures where converged theoretical results can be obtained in 3D. In our work for 3D lattices, we have entered the region where converged theoretical calculations are unavailable and quantum simulation manifests its usefulness.

While we successfully demonstrate the lowest temperature achieved in the FHM in our 1D optical lattice experiment, there is still room for reaching even lower temperatures, for example, by engineering spatial redistribution of entropy.

The STO measurement presented here is also applicable to spin-imbalanced cases by introducing proper oscillation functions. On the other hand, the spin structures measured in this work are limited to the SU(2)-type nearest-neighbour singlets and triplets. In general SU(N) systems, more nontrivial spin states arise. For example, the SU(N) singlet given by the fully antisymmetric combination of $N$ spins plays an essential role in SU(N) antiferromagnets. Probing such multi-spin entanglement will be an important experimental challenge. Measuring the long-range correlations is also of interest. One of the most important questions that has not yet been answered is whether the long-range ordering persists in the SU(N) system. Measuring long-range correlations will be feasible by using a quantum gas microscope with a spin-selective detection technique. State-of-the-art numerical and analytic calculations, with the use of approximations, have proposed a variety of possible ground states such as flavour-ordered patterns and valence bond solids, among others. Experiments are now poised to discriminate finite-temperature analogues of such proposed states.

**Online content**

Any methods, additional references, Nature Research reporting summaries, source data, extended data, supplementary information, acknowledgements, peer review information; details of author contributions and competing interests; and statements of data and code availability are available at https://doi.org/10.1038/s41567-022-01725-6.

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Methods

Sample preparation. A degenerate Fermi gas of $^{173}$Yb is prepared by evaporative cooling in a crossed dipole trap operating at 532 nm. The optical lattice also has the wavelength 532 nm and the simple cubic geometry. The additional detection lattices at 1,064 nm along the $z$- and $x$-axes are used only for STO measurement.

In the main result obtained in Fig. 3, the optical lattices are ramped up to $s = (s_x, s_y, s_z) = (7.0, 7.0, 7.0)$ for the 3D cubic lattice, $(6.1, 20.0, 6.1)$ for the 2D $(x-z)$ square lattice and $(20.0, 20.0, 5.0)$ for the 1D $(x$-chain) lattice. Here, $s_x$, $s_y$, and $s_z$ are the lattice depths in units of the recoil energy $s = h^2/(2m_{1s}a^3)$. To improve the spatial overlap, the atom cloud density is increased by evaporative cooling up to a $10\%$ of the trap depth.

The dipole trap together with the optical lattice creates an overall harmonic potential for the sample, whose trap frequencies are $(\omega_x, \omega_y, \omega_z) = 2\pi \times (102.4, 44.5, 155.0)$ Hz for the 3D lattice, $2\pi \times (105, 49, 158.0)$ Hz for the 2D lattice and $2\pi \times (107, 54, 162.0)$ Hz for the 1D lattice. The principal axes of the trap $x'$ and $y'$ are tilted by 45° from the lattice axes $x$ and $y$, within the horizontal plane. For the experiment shown in Extended Data Fig. 2, the trap frequency depends weakly on $U/\hbar$ with the variations within $1\%$.

The entropies of atomic gases are calculated numerically using the temperature obtained by fitting the Thomas–Fermi distribution to time-of-flight images of non-interacting gases. The effect of interaction during cloud expansion causes an additional systematic error in the entropy, which is estimated to be smaller than 1% of the PA rate and the correction to $N(t)$ is typically 1%. In the SU(2) case, the STO is a simple sinusoidal and the analogous expressions are

$$\begin{align*}
P_t &= \frac{1}{N_{\text{tot}}} \left[ N_{\text{tot}} - D + a - b \right], \\
P_0 &= \frac{1}{N_{\text{tot}}} \left[ N_{\text{tot}} - D - a - b \right].
\end{align*}
$$

An atom with specific $m_f$ can show STOs with two possible frequencies. With OSG separation, the time evolution of the atom number in each separated cloud $N_{m_f}$ is described by the two-frequency oscillation

$$N_{m_f}(t) = -a \exp(-\zeta t) \cos \omega_{m_f}(t) + b,$$

with oscillation frequencies

$$\omega_{m_f}(t) = \left\{ \begin{array}{ll}
(\omega_1, 3\omega_1) & |m_f| = 1/2 \\
(\omega_2, 3\omega_2) & |m_f| = 3/2 \\
(2\omega_3, 3\omega_3) & |m_f| = 5/2.
\end{array} \right.$$  

Numerical calculations for homogeneous systems. DQMC and ED calculations are used to obtain the values of the thermodynamic quantities, including the density, entropy and nearest-neighbor correlation function for homogeneous systems. These results are used to compute the properties for the trapped system using the LDA, which is described below.

ED results were obtained in $L$-site chains by performing full diagonalization over a reduced Hilbert space (described below) and using finite-size scaling. For computational efficiency, we exploit two aspects of the SU(N) symmetry. Particle number conservation for each spin flavour

$[N_{\sigma}, H] = 0$

with $N_{\sigma} = \sum_i n_{i\sigma}$ and the translation symmetries allow us to block-diagonalize the Hamiltonian. Furthermore, we exploit the spin permutation symmetries

$[S^z_{\sigma}, H] = 0, \quad \forall \sigma, \tau = 1, \ldots, N$

with

$S^z_{\sigma} = \sum_i S^z_{\sigma i} = \sum_i n_{i\sigma}$,

which relate many of the sectors of the Hamiltonian, and therefore one needs to diagonalize only one representative from each sector.

In addition to the (exact) symmetries, we exploit a basis state truncation, which we converge systematically. First, the Hilbert space only includes states with total particle number less than or equal to a fixed particle number $N_{\text{max}}$. Second, it omits states that total on-site energy is the energy associated with the presence of multiple occupancies in the cluster is larger than $E_{\text{var}}$. We present results obtained from $N_{\text{max}} = L + 1$ and $E_{\text{var}} = U$ for $L = 5$ and $N_{\text{max}} = L$ for $L = 8$. Extended Data Fig. 3 shows that the results for the STO amplitude versus entropy with these truncations are converged to $10^{-4}$.

DQMC results for 4×4 square and 4×4×4 cubic lattices were obtained by introducing $N(N-1)/2$ auxiliary Hubbard–Stratonovich fields, one for each interaction term $n_n n_n$. Note that previous works applied DQMC to the half-filled SU(2N) FHM using a different, discrete complex Hubbard–Stratonovich decomposition. Following our new approach, DQMC calculations for fillings below 1.5 particles per site at $U/\hbar = 15.3$ can be obtained reliably for temperatures $k_B T \geq t$. At lower temperatures, correlation functions become inaccessible to DQMC owing to sign and ergodicity problems. DQMC data were obtained for five different random seeds, each with 8,000 sweeps through the lattice and the $N(N-1)/2$ auxiliary fields for equilibration and 100,000 sweeps for measurements. The inverse temperature was discretized as $\beta = L \pi \tau$ with a Trotter step of $\tau = 0.025T$. Results are obtained in $\mu - T$ grids with $d\mu = 0.25 \tau$ and $dT$ given by the Trotter step for all integers $\mu \geq 2$. These results are linearly interpolated before computing the entropy and using the LDA. The entropy per site is computed as the integral of the specific heat, which by thermodynamic relations can be rearranged to

$$s(\mu, T) = N \log(2) + \left( \frac{f(\mu, T)}{T} \right) - \int_T^\infty \left( f(\mu, T) \right) dT,$$
\[ N_{\text{ptcl}} = \int \frac{d^3r}{a^3} m(\mu_0 - V(r), T), \]  
\[ S = \int \frac{d^3r}{a^3} s(\mu_0 - V(r), T), \]

where \( n/a^2 \) and \( s/a^2 \) are the density and entropy density calculated for the homogeneous system. The variables that can be measured experimentally are \( N_{\text{ptcl}} \) and \( S \) rather than \( \mu_0 \) and \( T \). But given the homogeneous functions \( m(\mu, T) \) and \( s(\mu, T) \), then \( \mu_0 \) and \( T \) can be obtained from \( N_{\text{ptcl}} \) and \( S \) by solving equations (15) and (16) numerically.

As derived below, the STO amplitude \( A \) and imbalance \( I \) are related to the correlation \( C_{\text{latt}} \), defined in equation (4), and to the correlation \( (n)(n+1) \) by

\[ A = -\frac{1}{N_{\text{ptcl}}} \left[ \frac{\Theta}{\text{latt}} \right], \]
\[ I = \frac{2A}{N_{\text{ptcl}}} \left[ \frac{\Theta}{\text{latt}} \right] + A \]

in the LDA, where we define

\[ [O] \left[ \text{latt} \right] = \int \frac{d^3r}{a^3} (O(\mu(r), T)). \]

In practice, we calculate plots of observable versus \( T \) or \( S \) as follows. First, we calculate a list of points \( (T, \mu) \) where \( \mu \) is obtained by solving equation (15) for \( T \) and the particle number \( N_{\text{ptcl}} \) measured in experiment. Then, for each such obtained \( (T, \mu) \), we calculate \( S \) and other trap-summed observables of interest. In this way, we plot trap-summed observables as functions of \( T \). Details on the grid used and discretization error introduced are given below.

**Trap geometry.** Owing to the large atomic mass of Yb, the effect of gravity is severe for our optical trap, especially in the final stage of evaporative cooling (Extended Data Fig. 4a). To include the anharmonic effect in our LDA calculation, we evaluate the density of states (DOS) defined as

\[ D(E) = \frac{\Theta}{\text{latt}} \sum_{\text{lattice sites}} (E - \tilde{V}(r)), \]

where \( \tilde{V}(r) \) is the full external potential at the site \( i \) except the periodic part forming optical lattices. Note that this DOS function becomes exact only in the atomic limit \( \tilde{r} \rightarrow 0 \) but is always valid for use in the LDA integral described below. Trap-summed observables are calculated using equations (15)–(19). These integrals over space are then rewritten as integrals over energy with the DOS:

\[ [O] \left[ \text{latt} \right] = \int dE D(E) (O(\mu_0 - E, T)). \]

In the harmonic approximation, the DOS is given by

\[ D(E) = \frac{2\pi \hbar^2}{a^3} \left( \frac{2}{m_0} \right)^{1/2} E^{1/2}, \]

where \( \hbar \) is the geometric mean of the trap frequencies.

**STO amplitude and imbalance.** In the limit where there are no multiple occupations, the populations in the singlet and triplet states \( P_{s,s}^{\mu_0}(i) \) and \( P_{s,t}^{\mu_0}(i) \) for an STO with spin components \( s \) and \( t \) in the dimer located on sites \( i \) and \( i+1 \) are given by the expectation value of the projection operators

\[ P_{s,s}^{\mu_0}(i) = \frac{1}{2} (\langle c_{i,s} c_{i+1,s} - c_{i,s}^\dagger c_{i+1,s}^\dagger \rangle \times (c_{i+1,s} c_{i,s} - c_{i+1,s} c_{i,s}^\dagger)), \]
\[ P_{s,t}^{\mu_0}(i) = \frac{1}{2} (\langle c_{i,s} c_{i+1,t} + c_{i+1,s} c_{i,t} \rangle \times (c_{i+1,s} c_{i,t}^\dagger + c_{i+1,t} c_{i,s}^\dagger)). \]

Note that these refer to SU(2) singlets involving components \( s \) and \( t \) rather than SU(3) singlets. It is useful to introduce 1/2-1/2 operators \( S_{\sigma}(i) = [n_{\sigma}(i) - n_{\sigma}(i)/2 \] for the pair of states \( \sigma \) and \( \tau \). By the SU(N) symmetry, the population difference and sum are equal to

\[ P_{s,s}^{\mu_0}(i) - P_{s,t}^{\mu_0}(i) = -4(S_{s}^{\mu_0}(i) S_{t}^{\mu_0}(i+1)), \]
\[ P_{s,s}^{\mu_0}(i) + P_{s,t}^{\mu_0}(i) = + \frac{1}{2} (n(i)(n(i+1) + 1)) - 2(S_{s}^{\mu_0}(i) S_{t}^{\mu_0}(i+1)). \]

The fractions of atoms forming singlets \( P_s = N_s/N_{\text{ptcl}} \) and triplets \( P_t = N_t/N_{\text{ptcl}} \) are obtained from a sum over each dimer in the lattice, or equivalently (1/2)\( \sum_{\sigma=\tau} \), and all the possible \( s - \tau \) spin pairs,

\[ P_s = \frac{2}{N_{\text{ptcl}}} \left[ \frac{1}{2} \sum_{\sigma=\tau} \left( \frac{1}{2} \sum_{\mu_0} P_{s,s}^{\mu_0}(i) \right) \right] \]
\[ P_t = \frac{2}{N_{\text{ptcl}}} \left[ \frac{1}{2} \sum_{\sigma=\tau} \left( \frac{1}{2} \sum_{\mu_0} P_{s,t}^{\mu_0}(i) \right) \right]. \]

Therefore, the global STO amplitude is

\[ A = P_s - P_t = \sum_{\sigma=\tau} \sum_{\mu_0} \frac{-4(S_{\sigma}(i) S_{\tau}(i+1))}{2N_{\text{ptcl}}} \]

which in terms of the \( n_s(i) \) is

\[ A = \sum_{\sigma=\tau} \sum_{\mu_0} C_{O\sigma}(i) \]

The STO imbalance \( I \) is defined as

\[ I = \frac{P_s - P_t}{P_s + P_t}, \]

so

\[ I = \frac{2A}{N_{\text{ptcl}}} \sum_{\sigma=\tau} \sum_{\mu_0} \frac{C_{O\sigma}(i)(n(i)(n(i+1)))}{C_{O\sigma}(i)} \]

where \( (n)(n+1) \) is the density–density correlation function. Equations (29)–(31) directly yield equations (17) and (18).

**Thermometry in 1D.** Extended Data Fig. 1 shows how we determine the lowest temperature achieved in the 1D experiments (\( \pm 0.096 \pm 0.054 \pm 0.030 \)). Estimates based on \( A \) rather than \( I \) give a similar result. The estimate based on the lowest entropy before lattice loading predicts a somewhat lower temperature, although still consistent within error bars. A small increase in temperature could result from non-adiabatic effects during the lattice loading. Extended Data Fig. 2 shows the interaction dependence of the spin correlations. The tendency towards larger discrepancy between theory and measurement with larger interactions (equivalent to deeper lattice depths) suggests that heating is important for deeper lattices.

**ED error estimates.** Errors for the ED results arise from two sources: finite-size error and truncation of the Hilbert space using the on-site energy and maximum particle number \( p_0 \) pa. Extended Data Fig. 5 presents the normalized STO amplitude and imbalance for SU(2) and SU(6) in 1D for different system sizes of \( L = 5-8 \), as well as the finite-size extrapolation. Results in the main text are presented after finite-size scaling at fixed entropy per particle, which is performed.
by fitting the results for $L = 5-8$ to $O_L = O_\infty + m/L$ with $O_\infty$ and $m$ as fitting parameters. Validity of the Hilbert space truncation is tested by varying the energy cut-off $E_m$ as well as the maximum particle number $N_{\text{max}}$. Extended Data Fig. 3 demonstrates that, for the interaction strengths considered herein, the truncation is extremely accurate, with no visible differences for any parameters.

**DQMC error estimates.** The DQMC results have several sources of error, which are estimated and presented in Extended Data Table 1 for SU(6) and $U/t = 15.3$ and in Extended Data Table 2 for SU(3) at $U/t = 8$. All error estimates are presented after the adiabatic loading calculation obtained by calculations for a $4 \times 4 \times 4$ lattice at $k_B T/t = 1$ unless explicitly stated otherwise. In this section, we briefly discuss how each error source was estimated.

The largest and most difficult to quantify error comes from finite-size effects. As a proxy, we estimate finite-size effects in two different ways. Our first estimate is a spot check comparison between the $3 \times 3 \times 3$ and $4 \times 4 \times 4$ systems at fixed $T/t$ and density. We obtain $C_{\text{O}(3 \times 3 	imes 3) - 4 \times 4 \times 4} = -0.096 \pm 0.004$ and $C_{\text{O}(3 \times 3 \times 3) - 5 \times 5 \times 5} = -0.125 \pm 0.005$ at the lowest temperature ($T/t = 1$) for a homogeneous system at $(n) = 1$, and this error decreases rapidly with increasing temperature. Note that this error may be dominated by the error of the smaller, $3 \times 3 \times 3$ system rather than reflecting the smaller error in the $4 \times 4 \times 4$ system. Our second estimate is by studying 2D, and taking the difference between the $4 \times 4$ results and the $6 \times 6$ results for the full computations of LDA-averaged observables. Larger system sizes, in particular in 3D, remain inaccessible at present.

The inverse temperature discretization error is estimated as the difference of the results obtained with Trotter steps of $\Delta \tau = 0.025$ and $\Delta \tau = 0.05$.

The entropy per site $S$ at temperature $T$ is given by equation (14). Errors in the calculation of $S$ arise from the finite value of the temperature cut-off $T_m$. This error was estimated in the homogeneous case by comparing the results obtained with $k_B T_m = 500, 800$ and 1,000.

Errors in numerical integration procedures such as the LDA summing of observables in the trap and the computation of the entropy are estimated by varying the coarseness of the $\mu - T$ integration grids. Such estimations were obtained by coarsening them by a factor of two and comparing the results.

Statistical errors are presented for both the homogeneous case and after adiabatic loading for five different random seeds. These errors are presented as the s.e.m.

**Data availability**

All the data presented in this paper are available from the corresponding author upon reasonable request.

**Code availability**

The mathematical codes that support the findings of this study are available from the corresponding author upon reasonable request.

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**Author contributions**

S.T., N.N. and Y. Takasu carried out experiments. S.T. analysed the data. Y.K. gave advice on experiments from the theoretical viewpoint. Y. Takahashi conducted the whole experiment. E.I.-G.-P. developed the SU(N) DQMC code extended from R.T.S.’s SU(2) code, performed the DQMC calculations, many ED calculations and the LDA calculations with ED and DQMC results, and carried out the theoretical data analysis. H.-T.W. developed the ED code and performed many of the ED calculations. R.T.S. and K.R.A.H. conceived and supervised the theoretical calculations. E.I.-G.-P., H.-T.W., R.T.S. and K.R.A.H. all contributed to interpreting the theory and theory–experiment comparisons. All the authors contributed to preparing the manuscript. S.T. and E.I.-G.-P. contributed equally to this work.

**Competing interests**

The authors declare no competing interests.

**Additional information**

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Extended Data Fig. 1 | Temperature of a 1D SU(6) Fermi gas at $U/t = 15.3$. The vertical dashed lines indicate the range of the largest experimentally measured STO imbalance in 1D that is consistent with error bars. The temperature of this datapoint is inferred from the finite-size scaling curves and the results are summarized in panel (d). The fss error is a conservative estimate of the finite-size error, the difference between the finite-size scaled results and the $L = 8$ site chain. The exp error comes from the experimental uncertainty on the correlations.
Extended Data Fig. 2 | Interaction dependence of the nearest neighbor correlations. Behavior of (a) STO amplitude and (b) singlet-triplet imbalance in 1D and 3D lattices are shown. Experimental data is shown for SU(6) systems with initial entropy $S/N_{\text{ptcl}}k_B = 1.4 \pm 0.1$. The error bars are extracted from the error of fit in the analysis of the STO signal. Solid lines are the result of exact diagonalization calculations for $S/N_{\text{ptcl}}k_B = 1.4$, and the error bars correspond to the sum in quadrature of the finite-size error and the basis-state truncation error. The inset presents the entropy per particle extracted by fitting it to reproduce the experimentally measured spin correlations. Results saturate at $S/N_{\text{ptcl}}k_B = 1.818 \pm 0.005$. Error bars in the inset come from the experimental uncertainty on the correlations.
Extended Data Fig. 3 | Normalized STO amplitude for an SU(6) Fermi gas in an $L=5$ site chain with $U/t=15.3$ for different truncations of the Hilbert space. Basis states with an on-site energy larger than the energy cutoff $E_{\text{cut}}$, as well as those that exceed the maximum particle number $N_{\text{max}}$ are disregarded. There is no visible difference between calculations. The inset shows the absolute value of the difference between the $E_{\text{cut}} = U, N_{\text{max}} = 5$ and $E_{\text{cut}} = 2U, N_{\text{max}} = 5$ curves.
Extended Data Fig. 4 | Trap anharmonicity. (a) Full external potential (optical + gravity) profile along the direction of gravity $z$. The shaded region is excluded from the calculation of DOS. (b) Density of states calculated from the external potential for the 3D cubic geometry. The corresponding harmonic approximation is also shown. The atoms are sensitive only to the density of states for $E/t \lesssim 10$. 
Extended Data Fig. 5 | Finite-size scaling in 1D. Normalized STO amplitude and imbalance for SU(2) and SU(6) Fermi gases in $L$-site chains and the results after finite-size scaling (fss) for $U/t = 15.3$. The inset in panel (b) illustrates the finite-size scaling procedure.
### Extended Data Table 1 | Error estimates for the DQMC calculation at $U/t = 15.3$.

Errors are presented at $k_B T/t = 1$. Most errors decrease with increasing temperature. The top two rows estimate errors by considering homogeneous systems as follows: “Finite $T_{\text{cut}}$” is the error by a non-infinite value of $T_{\text{cut}}$ in entropy integrations estimated by the difference of $k_B T_{\text{cut}} = 1000$ and 500. “Statistical” estimates is the standard error of the mean, taken at its largest value over all $\mu$ and $T$ considered. The bottom 5 rows come from results after adiabatic loading in the trap, as follows. “Finite size (2D)” is the finite-size error estimated by the difference between $A(S)$ in $4 \times 4$ and $6 \times 6$ geometries, “Trotter-step” is the Trotter error estimated by the difference of $A(S)$ for Trotter step size $\Delta \mu = 0.05$ and 0.025, “$\mu$-grid coarseness” and “$T$-grid coarseness” are the estimates of the errors associated with discretizing $\mu$ and $T$ by taking the difference of the result after doubling the grid spacing, and “Statistical (adiabatic loading)” is the standard error of the mean of the DQMC.

| Error source (homogeneous, worst case over all $\mu$ and $T$) | $S$ vs $T$ | $A$ vs $T$ | $I$ vs $T$ |
|-------------------------------------------------------------|------------|------------|------------|
| Finite $T_{\text{cut}}$                                    | $1.3 \times 10^{-4}$ | $-$         | $-$         |
| Statistical                                                 | $1.2 \times 10^{0}$  | $1.8 \times 10^{-1}$ | $8.6 \times 10^{-2}$ |
| Error source (in the trap)                                  | $S$ vs $T$ | $A$ vs $S$ | $I$ vs $S$ |
| Finite size (2D)                                            | $1.8 \times 10^{-2}$ | $1.1 \times 10^{-2}$ | $2.4 \times 10^{-2}$ |
| Trotter-step                                                | $1.8 \times 10^{-2}$ | $4.6 \times 10^{-3}$ | $9.5 \times 10^{-3}$ |
| $\mu$ grid coarseness                                       | $6.9 \times 10^{-3}$ | $7.2 \times 10^{-3}$ | $1.5 \times 10^{-2}$ |
| $T$ grid coarseness                                         | $1.4 \times 10^{-2}$ | $2.4 \times 10^{-3}$ | $5.3 \times 10^{-3}$ |
| Statistical (adiabatic loading)                             | $1.0 \times 10^{-2}$ | $1.6 \times 10^{-3}$ | $3.2 \times 10^{-3}$ |
Extended Data Table 2 | Error estimates for the different error sources involved in the DQMC calculation for $U/t = 8$ and $N = 3$. Row labels are the same as in Extended Data Table 1. The first three rows are for homogeneous systems while the last is for the $A(S)$ after adiabatic loading. For homogeneous system results, we report the largest error in the whole range of temperatures/entropies considered. The $T$ grid coarseness error for $S$ vs $T$ monotonically increases from $2.0 \times 10^{-2}$ at $k_B T/t = 0.64$ to the value reported in the table, $1.3 \times 10^{-1}$, at $k_B T/t = 4$.

| Error source | $S$ vs $T$ | $A$ vs $S$ | $I$ vs $S$ |
|--------------|-----------|-----------|-----------|
| Trotter-step | $3.2 \times 10^{-2}$ | $7.8 \times 10^{-4}$ | $2.1 \times 10^{-3}$ |
| $\mu$ grid coarseness | $7.8 \times 10^{-4}$ | $1.6 \times 10^{-4}$ | $5.2 \times 10^{-4}$ |
| $T$ grid coarseness | $1.3 \times 10^{-1}$ | $1.8 \times 10^{-3}$ | $4.9 \times 10^{-3}$ |
| Statistical (adiabatic loading) | $2.0 \times 10^{-4}$ | $5.0 \times 10^{-5}$ | $1.2 \times 10^{-4}$ |