

Realizing Exactly Solvable SU(N) Magnets with Thermal Atoms

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We show that n thermal fermionic alkaline-earth atoms in a flat-bottom trap allow one to robustly implement a spin model displaying two symmetries: the S_n symmetry that permutes atoms occupying different vibrational levels of the trap and the $SU(N)$ symmetry associated with N nuclear spin states. The high symmetry makes the model exactly solvable, which, in turn, enables the analytic study of dynamical processes such as spin diffusion in this $SU(N)$ system. We also show how to use this system to generate entangled states that allow for Heisenberg-limited metrology. This highly symmetric spin model should be experimentally realizable even when the vibrational levels are occupied according to a high-temperature thermal or an arbitrary non-thermal distribution.

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The study of quantum magnetism with ultracold atoms [1, 2] promises to give crucial insights into a range of many-body phenomena from frustrated magnets and quantum spin liquids [3] to many-body localization [4] and quantum quenches [5]. A typical approach to implementing a quantum magnet with ultracold atoms relies on preparing a Mott insulator in an optical lattice, where the internal states of atoms on each site define the effective spin [1]. Virtual hopping processes to neighboring sites and back then give rise to effective superexchange spin-spin interactions. Because the superexchange interactions are very weak (\ll kHz) [1], it is a significant challenge in experimental cold atom physics to achieve temperatures low enough to access superexchange-based quantum magnetism.

Since ultracold atoms can be prepared in specific internal (i.e. spin) states with extremely high precision, spin temperatures that can be realized are much lower than the experimentally achievable motional temperatures. It is therefore tempting to circumvent the problem of high motional temperature by constructing a spin model in such a way that the motional and spin degrees of freedom are effectively decoupled. In this Letter, we provide a recipe for such a decoupling and hence for realizing spin models with thermal atoms. The basic idea can be understood as follows.

The first crucial ingredient is to depart from second-order superexchange interactions and use contact interactions to first order [6–15]. As shown in Fig. 1(a), this can be achieved if all atoms sit in different orbitals of the same anharmonic trap and remain in these orbitals throughout the evolution, which is a good approximation for weak interactions [6–8, 13, 14]. In that case, the occupied orbitals play the role of the sites of the magnet. However, because of high motional temperature in such systems, every run of the experiment typically yields a different set of populated orbitals and hence a differ-

ent spin Hamiltonian [13]. Thus, unless the dynamics are constrained to states symmetric under arbitrary exchanges of spins [13], every run of the experiment would lead to different spin dynamics.

The second crucial ingredient of our proposal is therefore required to decouple spin and motion: the use of an infinite one-dimensional square-well potential as the anharmonic trap, with the motion frozen along the other two directions. In that case, being proportional to the squared overlap of pairs of distinct occupied orbitals, all interaction terms in the spin Hamiltonian \hat{H} have the same strength. Therefore \hat{H} is independent of which orbitals are occupied, leading to spin-motion decoupling and temperature independent predictions, as well as opening up the possibility of precise control. Moreover, since \hat{H} is invariant under any relabeling of the n occupied orbitals, \hat{H} has S_n permutation symmetry.

Alkaline-earth atoms enrich the symmetry. In such atoms, the vanishing electronic angular momentum J in the electronic clock states $g = {}^1S_0$ and $e = {}^3P_0$ results in

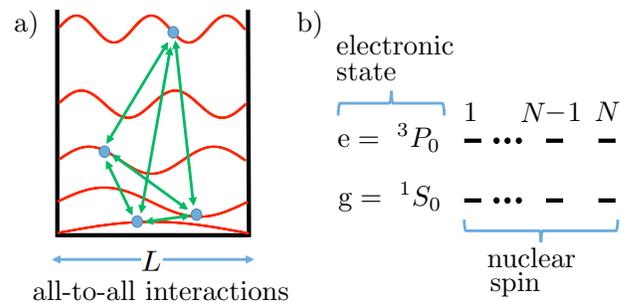


FIG. 1: (a) Contact interactions between atoms in the orbitals of a one-dimensional infinite square well of width L are all-to-all with equal strength. (b) Thanks to the nuclear spin I , each of the electronic clock states g and e of fermionic alkaline-earth atoms can offer N degenerate states, with $N \leq 2I + 1$.

the decoupling of the nuclear spin I from J [Fig. 1(b)]. This endows \hat{H} with an additional $SU(N)$ spin-rotation symmetry, where N can be tuned between 2 and $2I + 1$ by choosing the initial state [16–21]. Restricted to g , \hat{H} is just the sum of spin-swaps over all pairs of occupied orbitals and can be diagonalized in terms of irreducible representations of the group of symmetries $G = S_n \times SU(N)$.

Motional-temperature-insensitive spin models can also be realized using *long-range* interactions between ions in Paul traps [22] and between molecules [23–26] or Rydberg atoms [27] pinned at different sites of an optical lattice. In contrast, our proposal relies on *contact* interactions, which are crucial for probing fermionic statistics and hence for realizing $SU(N)$ -symmetric spin models.

We first study spin diffusion [26, 28, 29] in a system of g atoms only. Due to crucial use of representation-theoretic techniques, our calculations are exponentially faster than naive exact diagonalization. We then present a protocol that employs both g and e states to create Greenberger-Horne-Zeilinger (GHZ) states [30], which could be used to approach the Heisenberg limit for metrology and clock precision [31].

Spin Hamiltonian.—A single mass- M fermionic alkaline-earth atom (for now, in its ground electronic state g) trapped in a 1D spin-independent potential $V(x)$ has real orbitals $\phi_j(x)$ with energies E_j satisfying $[-(1/2M)\partial^2/\partial x^2 + V(x)]\phi_j(x) = E_j\phi_j(x)$ (setting $\hbar = 1$). The operator \hat{c}_{jp}^\dagger creates an atom from the vacuum $|vac\rangle$ in $\phi_j(x)$ with nuclear spin state $p \in 1, 2, \dots, N$. For n identical atoms in the same potential with contact s -wave interactions, the Hamiltonian is $\hat{H} = \sum_{jp} E_j \hat{c}_{jp}^\dagger \hat{c}_{jp} + \sum_{p < q} \sum_{jkj'k'} U_{jkj'k'} \hat{c}_{jp}^\dagger \hat{c}_{j'p}^\dagger \hat{c}_{kq} \hat{c}_{k'q}$, where $U_{jkj'k'} = 2\omega_\perp a_{gg} \int_{-\infty}^{\infty} dx \phi_j(x) \phi_k(x) \phi_{j'}(x) \phi_{k'}(x)$, a_{gg} is the 3D-scattering length, and a potential with frequency ω_\perp freezes out transverse motion.

To obtain the desired highly symmetric Hamiltonian, we specialize to the case where $V(x)$ is a width- L infinite square well, with well-known eigenstates $\phi_j(x) = \sqrt{2/L} \sin(j\pi x/L)$ for $0 \leq x \leq L$, with energy $E_j = (\pi j/L)^2/2M$. Then $U_{jkj'k'}$ is zero unless (i): $(j \pm k) = \pm(j' \pm k')$. To first order in the interaction, we can also set $U_{jkj'k'} \rightarrow 0$ unless $\sum_{jp} E_j \hat{c}_{jp}^\dagger \hat{c}_{jp}$ is conserved, which occurs when (ii): $j^2 + k^2 = j'^2 + k'^2$. Conditions (i) and (ii) are both satisfied if and only if $(j', k') = (j, k)$ or $(k', j') = (j, k)$. As the system conserves orbital occupancies it can be described by a spin model. Assuming orbitals are at most singly occupied ($\hat{n}_j = \sum_p \hat{c}_{jp}^\dagger \hat{c}_{jp} \leq 1$ for all j) [54], the spin Hamiltonian is:

$$\hat{H} = -U \sum_{j < k} \hat{s}_{jk}, \quad (1)$$

where $\hat{s}_{jk} \equiv \sum_{pq} \hat{c}_{jp}^\dagger \hat{c}_{jq} \hat{c}_{kq}^\dagger \hat{c}_{kp}$ swaps spins j and k , and the sum is over occupied orbitals. Crucially, $U \equiv 4\pi a_{gg} \omega_\perp / L$ is independent of j and k . We dropped a

constant $\sum_j E_j + n(n-1)U/2$, which will have no effect on spin dynamics. For a fixed set of occupied orbitals, \hat{H} has N^n basis states $|p_1, p_2, \dots, p_n\rangle$ with $p_j \in 1, \dots, N$.

Exact eigenenergies and eigenstates.—For $N = 2$, the spin-swap can be written in terms of the Pauli operators: $\hat{s}_{jk} = 1/2 + (\hat{\sigma}_j^x \hat{\sigma}_k^x + \hat{\sigma}_j^y \hat{\sigma}_k^y + \hat{\sigma}_j^z \hat{\sigma}_k^z)/2$, allowing Eq. (1) to be written as $\hat{H} = -U \left[\vec{S}^2 + \frac{n}{4}(n-4) \right]$, where $\vec{S} = \frac{1}{2} \sum_j \vec{\sigma}_j$. The eigenstates of \hat{H} for $N = 2$ are the well-known Dicke [32] states $|S, S_z, k\rangle$, with energies $E(S) = -U \left[S(S+1) + \frac{n}{4}(n-4) \right]$. The quantum number k labels distinct states with the same \vec{S}^2 and \hat{S}^z eigenvalues. We now describe the general case for arbitrary N , but defer derivations and detailed explanation to Ref. [33].

Equation (1) has two obvious symmetries: permutations in S_n of the n occupied orbitals, and application of the same unitary in $SU(N)$ to all of the spins giving a group $G = SU(N) \times S_n$ of symmetries. From Schur-Weyl duality [34], we conclude that for each integer partition $\vec{\lambda} = (\lambda_1, \lambda_2, \dots, \lambda_N)$ such that $\sum_i \lambda_i = n$ and $\lambda_{i+1} \leq \lambda_i$, there is a subspace of constant energy $E(\vec{\lambda})$. The $\vec{\lambda}$ -subspaces (called irreducible representations of G) are orthogonal and span the full Hilbert space.

A *Young diagram* is a pictorial representation of $\vec{\lambda}$ consisting of a row of λ_1 boxes above a row of λ_2 boxes, which is above a row of λ_3 boxes etc. It is also useful to define $\vec{\gamma} = (\gamma_1, \gamma_2, \dots, \gamma_{\lambda_1})$ as the column heights of the Young diagram $\vec{\lambda}$. Figure 2(a) shows an example with $n = 7$ and $N = 3$.

Now we show how to create an eigenstate in any $\vec{\lambda}$ -subspace. First consider the basis state: $|T\rangle \equiv |1, 2, \dots, \gamma_1\rangle |1, 2, \dots, \gamma_2\rangle \dots |1, 2, \dots, \gamma_{\lambda_1}\rangle$, which is chosen by associating orbitals with boxes of the Young diagram as in Fig. 2(b), and putting those orbitals in spin states as in Fig. 2(c). We form $|\vec{\lambda}\rangle$ (which is one of many [33] eigenstates in the $\vec{\lambda}$ -subspace) by antisymmetrizing $|T\rangle$ over orbitals associated with boxes in each column of $\vec{\lambda}$:

$$|\vec{\lambda}\rangle = |\mathcal{A}\{12\dots\gamma_1\}\rangle |\mathcal{A}\{12\dots\gamma_2\}\rangle \dots |\mathcal{A}\{12\dots\gamma_{\lambda_1}\}\rangle, \quad (2)$$

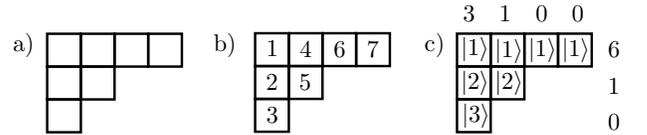


FIG. 2: (a) An example Young diagram $\vec{\lambda} = (4, 2, 1)$ (with $\vec{\gamma} = (3, 2, 1, 1)$) for $n = 7, N = 3$. (b) A labeling of boxes in Young diagram $\vec{\lambda}$ from 1 to n , increasing down columns, starting at the left. (c) Orbitals associated with boxes in the p th row of the Young diagram are put in spin state $|p\rangle$ to form basis state $|T\rangle = |1231211\rangle$ [spins ordered as in (b)], used to construct eigenstate $|\vec{\lambda}\rangle = |\mathcal{A}\{123\}\rangle |\mathcal{A}\{12\}\rangle |1\rangle$ with $E(\vec{\lambda})/(-U) = \sum_i \binom{\lambda_i}{2} - \sum_j \binom{\gamma_j}{2} = 6 + 1 + 0 - 3 - 1 - 0 - 0 = 3$.

where $\mathcal{A}\{\dots\}$ antisymmetrizes its argument, for example: $|\mathcal{A}\{123\}\rangle = |123\rangle + |312\rangle + |231\rangle - |132\rangle - |321\rangle - |213\rangle$. The normalization constant is fixed by $\langle \vec{\lambda} | \vec{\lambda} \rangle = \gamma_1! \gamma_2! \dots \gamma_{\lambda_1}!$. We see that the Young diagram associates symmetry with rows and antisymmetry with columns.

From $\hat{H}|\vec{\lambda}\rangle = E(\vec{\lambda})|\vec{\lambda}\rangle$ one can prove $E(\vec{\lambda})/(-U) = \sum_{i=1}^N \binom{\lambda_i}{2} - \sum_{j=1}^{\lambda_1} \binom{\gamma_j}{2}$: the number of ways of choosing two boxes in the same row of $\vec{\lambda}$, minus the number of ways of choosing two boxes in the same column [33]. This is in line with the intuition that the swap picks up $-U$ for each symmetric pair and $+U$ for each antisymmetric pair in the Young diagram. In terms of $\vec{\lambda}$,

$$E(\vec{\lambda}) = -\frac{U}{2} \sum_{i=1}^N (\lambda_i - 2i + 1) \lambda_i. \quad (3)$$

There is an equivalence for the $SU(2)$ case between Young diagram (λ_1, λ_2) and angular momentum quantum number S given by $S = (\lambda_1 - \lambda_2)/2 = (2\lambda_1 - n)/2$.

Spin diffusion dynamics.—Spin diffusion is the process by which evolution under a generic spin Hamiltonian causes initially ordered states to diffuse [26, 28, 29]. We take initial state $|\psi(0)\rangle = |1\rangle^{\otimes m_1} |2\rangle^{\otimes m_2} \dots |N\rangle^{\otimes m_N}$. Note that any computational basis state can be changed to this form by reordering occupied orbitals. We consider the time evolution of observable $\hat{Q} = \sum_{j=1}^{m_1} |1\rangle_j \langle 1|_j$: the number of the first m_1 orbitals in spin-state $|1\rangle$. The expectation of \hat{Q} evolves according to: $Q(t) \equiv \langle \psi(0) | e^{i\hat{H}t} \hat{Q} e^{-i\hat{H}t} | \psi(0) \rangle$.

Calculation of such a time evolution for a generic Hamiltonian requires diagonalization of a matrix, which scales exponentially with n (for fixed N). Using the symmetry of Hamiltonian (1) and the Wigner-Eckart theorem for $SU(N)$ we obtain an explicit sum (see Eq. (S11) in Ref. [33]) for $Q(t)$ in terms of Clebsch-Gordan and recoupling coefficients. For the case of $N = 2$, with initial state of $m_1 = m$ spin up and $m_2 = n - m$ spin down orbitals, using well-known closed forms for the Clebsch-Gordan and recoupling coefficients:

$$Q(t) = m + \sum_{S=|n-2m|/2+1}^{n/2} \gamma(S) [\cos(2SUt) - 1], \quad (4)$$

where $\gamma(S) = \frac{4S^2 - (n-2m)^2}{4S} \binom{n}{n/2+S} / \binom{n}{n-m}$. For $N > 2$, closed forms for the required coefficients are not known to the authors, but can be calculated efficiently using standard algorithms as in Ref. [35]. In Fig. 3, we compare the evolution of the same operator and total particle number for initial states with $N = 2$ spin states and $N = 3$ spin states. We see that oscillations are much less pronounced and spin diffusion occurs more fully (Q drops lower) for the latter state – consistent with the intuition that the initial state can diffuse into a much larger Hilbert space for $SU(3)$ than for $SU(2)$.

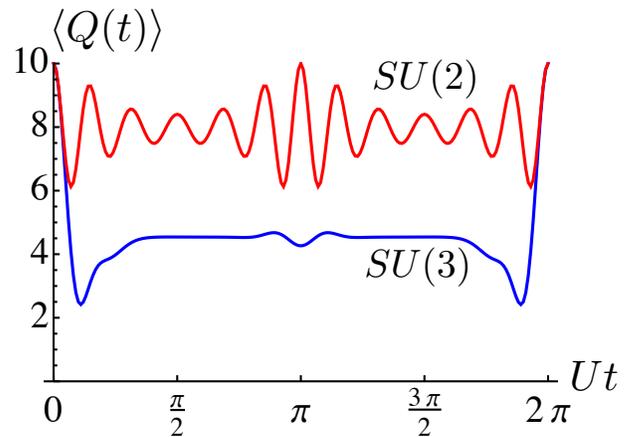


FIG. 3: Exact time evolution under \hat{H} of an operator $\hat{Q} = \sum_{j=1}^{10} |1\rangle_j \langle 1|_j$, which counts the number of the first ten orbitals in spin state $|1\rangle$. Two initial states are compared: $|1\rangle^{\otimes 10} |2\rangle^{\otimes 20}$ for $SU(2)$ and $|1\rangle^{\otimes 10} |2\rangle^{\otimes 10} |3\rangle^{\otimes 10}$ for $SU(3)$. Although the evolution is the same for short times, the $SU(3)$ case results in significantly more diffusion of spin state $|1\rangle$ out of the first four orbitals at later times. Since all $E(\vec{\lambda})$ are integer multiples of U , complete revival occurs at $Ut = 2\pi$. In the $SU(2)$ case, the oscillation is dominated by the smallest S in Eq. (4). This is consistent with the fact that for fixed S_z , the size of the eigenspaces decreases with S , causing overlap to be larger with subspaces of small S generically.

GHZ state preparation.—Highly entangled states could lead to short-term industrial applications in metrology, and long-term applications in quantum information. It is particularly timely to design ways for implementing entanglement-assisted clocks with alkaline-earth atoms [36, 37] since such atoms recently gave rise to the world’s best clock and nearly approached the quantum projection noise limit for disentangled atoms [38].

To create a GHZ state, we allow atoms in the excited electronic state e with an energy ω_{eg} above the ground electronic state g [see Fig. 1(b)]. First assume $N = 2$. An applied magnetic field adds Zeeman spin-splittings $B_g \neq B_e$ [39] to both g and e states. To first order in the interaction strength, the spin Hamiltonian is [33]:

$$\hat{H} = \hat{H}_{sp} + \sum_{\alpha < \beta} U_{\alpha\beta} \left(\hat{n}_{\alpha} \hat{n}_{\beta} - \sum_{j \neq k} \hat{c}_{j\alpha}^{\dagger} \hat{c}_{j\beta} \hat{c}_{k\beta}^{\dagger} \hat{c}_{k\alpha} \right). \quad (5)$$

The single-particle Hamiltonian is $\hat{H}_{sp} = \omega_{eg} \hat{n}_e + B_g(\hat{n}_{1g} - \hat{n}_{2g}) + B_e(\hat{n}_{1e} - \hat{n}_{2e})$, the sum $\alpha < \beta$ is over distinct pairs of $1g, 1e, 2g$ and $2e$, and the constants $U_{\alpha\beta}$ are derived in terms of (electronic-state dependent) scattering lengths [33]. Note that $\hat{n}_{1g}, \hat{n}_{2g}, \hat{n}_{1e}$ and \hat{n}_{2e} are separately conserved by Hamiltonian (5). As shown in Fig. 4, to create the n -particle GHZ state ($|1g1g..1g\rangle + |2g2g..2g\rangle$) from $|1g1g..1g\rangle$, three consecutive pulses should be applied:

1. Spatially inhomogeneous, weak, many-body $\pi/2$

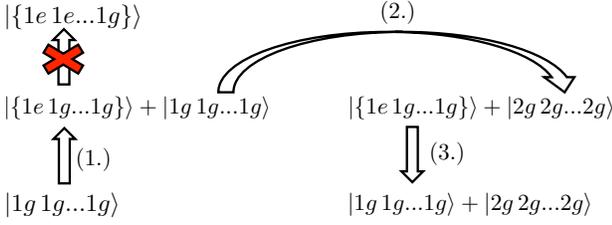


FIG. 4: The system is prepared in $|1g1g\dots1g\rangle$, and spatially inhomogeneous pulse (1.) results in an equal superposition of this state and $|\{1e1g\dots1g\}\rangle$, which has one e atom. An interaction blockade prevents coupling to states with two e atoms. Pulse (2.) flips the spins of the all- g state. The initial pulse is reversed in pulse (3.), resulting in the GHZ state.

pulse $e^{-i\nu_{eg}t} \sum_j \Omega_j^{eg} (|1e\rangle_j \langle 1g|_j + |2e\rangle_j \langle 2g|_j) + h.c.$
with frequency $\nu_{eg} = \omega_{eg} + (B_e - B_g) + nU_{1g1e}$.

2. Spatially uniform, weak, single-atom π pulse $e^{-i\nu_{12}t} \Omega^{12} \sum_j (|2g\rangle_j \langle 1g|_j + |2e\rangle_j \langle 1e|_j) + h.c.$ with frequency $\nu_{12} = 2B_g$.
3. Pulse 1, but for pulse area π , not $\pi/2$.

The frequency of the first pulse picks out an effective two-level system consisting of $|1g1g\dots1g\rangle$ and $|\{1e1g\dots1g\}\rangle \propto \sum_{jp} (\Omega_j^{eg} - \bar{\Omega}^{eg}) |1e\rangle_j \langle 1g|_j |1g1g\dots1g\rangle$ (we defined $\bar{\Omega}^{eg} \equiv \sum_j \Omega_j^{eg} / n$). The curly bracket notation signifies the state is a linear combination of $|1e1g\dots1g\rangle$ and permutations. No state $|\{1e1e\dots1g\}\rangle$ is coupled by pulse 1 because the first e atom blockades the addition of another by energy $2U_{1g1e}$ [33]. The second pulse has no effect on $|\{1e1g\dots1g\}\rangle$ because the e atom blockades transition to any state $|\{1e2g\dots1g\}\rangle$. The final pulse does not affect the $|2g2g\dots2g\rangle$ state because the pulse is off-resonant by energy of order $(B_e - B_g)$ [33]. Curiously, the fact that the interactions in our spin model have effectively infinite range makes our spins analogous to long-range interacting Rydberg atoms, for which a similar protocol exists for generating maximally entangled states [40]. Note that we have designed the protocol to have at most one e atom at any time, which avoids the potential problem of inelastic e - e collisions [41].

For integer m such that $N \geq 2^m$, it is possible to create m GHZ states provided one has sufficient control [42] over the nuclear spin states coupled by the pulses. We outline the procedure with $m = 2$. First create $(|11\dots1\rangle + |22\dots2\rangle)$ from $|1\dots1\rangle$ as above. Then repeat pulses 1 to 3, but apply $|p\rangle \mapsto |p+2\rangle$ (for $p = 1, 2$) instead of $|p\rangle \mapsto |p+1\rangle$ in pulse 2, resulting in $(|11\dots1\rangle + |22\dots2\rangle + |33\dots3\rangle + |44\dots4\rangle) = (|\downarrow\downarrow\dots\downarrow\rangle + |\uparrow\uparrow\dots\uparrow\rangle)(|\downarrow\downarrow\dots\downarrow\rangle + |\uparrow\uparrow\dots\uparrow\rangle)$, where we define $\{|1\rangle, |2\rangle, |3\rangle, |4\rangle\} \equiv \{|\downarrow\downarrow\rangle, |\downarrow\uparrow\rangle, |\uparrow\downarrow\rangle, |\uparrow\uparrow\rangle\}$. The process could be continued, where in the i th iteration pulse (2.) involves $|p\rangle \mapsto |p+2^i\rangle$ (for $p = 1, 2, 3, \dots, 2^i$). Several GHZ states can be used to create a single GHZ state of better fidelity via entanglement pumping [42, 43].

Experimental considerations.—We use the example of ^{87}Sr to describe how to experimentally access the physics we discuss in this Letter. We propose freezing out the x and y directions using a two-dimensional optical lattice potential formed by two magic-wavelength [44] orthogonal standing waves. The caps of all the resulting flat-bottom [45] tubes could be formed from two parallel sheets of magic-wavelength blue-detuned 390 nm light each in the x - y plane a distance L apart using a phase-imprinting spatial light modulator as in Ref. [46].

Taking $\omega_{\perp} = 2\pi \times 10$ kHz, and a similar cap barrier height, with $L = 10 \mu\text{m}$, and $a_{gg} = 5.1$ nm [47], one obtains $U = (4\pi a_{gg} \omega_{\perp}) / L \approx 2\pi \times 10$ Hz, and should be able to trap $\lesssim 20$ atoms in a single tube. One should ensure a trap length $L \gtrsim 10 \mu\text{m}$ to render the wall width (\sim optical wavelength) negligible. The validity of first-order perturbation theory in our derivation of Eq. (1) relied on sufficiently weak interactions: $U < 3\hbar^2(\pi/L)^2/M \approx 2\pi \times 30$ Hz for $L = 10 \mu\text{m}$. For the above parameters, taking a typical recombination rate constant $K_3 \approx 10^{-28}$ cm⁶/s for $n = 20$ particles, it should take approximately 1 second before a single particle is lost.

A build-up cavity opens the possibility of increased barrier height of the caps and ω_{\perp} , allowing one to trap many more atoms. In combination with subwavelength-resolution methods [42, 48–51] to create sharper walls and reduce L , one could bring U into the kHz range while keeping it below $3\hbar^2(\pi/L)^2/M$. It may also be possible to increase a_{gg} using optical Feshbach resonances [52], which would need to be carefully engineered to avoid destroying the $SU(N)$ symmetry.

The approximate magnitude of p -wave terms involving occupied orbitals j and k is $\pi^2(j^2 + k^2)(b_{gg}/L)^2(b_{gg}/a_{gg})U$, where b_{gg}^3 is the scattering volume for p -wave interactions. This remains small for $j, k < 300$, taking $b_{gg} \approx 3.9$ nm [18] for ^{87}Sr .

To observe spin diffusion, the most straightforward way of preparing the initial state and measuring observable \hat{Q} involves cooling a spin-polarized system to the limit where the lowest n orbitals are occupied. One can then address different orbitals either spatially with spin-changing pulses which only couple to certain orbitals, or energetically by temporarily transferring atoms to another electronic state subject to a different potential.

Outlook.—The proposed system opens a wide range of research and application avenues beyond those discussed above. For the case of $N = 2$, our $S_n \times SU(N)$ -symmetric Hamiltonian can be used for decoherence-resistant entanglement generation [53], a method whose generalization to $N > 2$ we postpone to future work. Furthermore, by comparing with the exact solutions presented here, one could verify the performance of the proposed experimental system as a quantum simulator. The system can then be used to reliably study more general regimes where complexity theory might rule out efficient classical solutions. In particular, deviations from the square-well po-

tential will break S_n (but not $SU(N)$) symmetry. This will for example lift the degeneracy of the most antisymmetric spin state (highest energy eigenspace for $U > 0$). Depending on how this degeneracy is lifted, exotic many-body states might arise. Finally, generalizations of our system to two and three dimensions can be envisioned, in which case additional potentials would need to be introduced to avoid mode-changing collisions [15].

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Supplemental Material for: “Realizing Exactly Solvable SU(N) Magnets with Thermal Atoms”

S1. USE OF SYMMETRY TO DIAGONALIZE HAMILTONIANS

Here we explain how to diagonalize the Hamiltonian by means of Schur’s lemma, attempting to minimize use of technical language.

Consider a group of unitary operators $G = \{\hat{U}_1, \hat{U}_2, \dots\}$ which commute with \hat{H} . Written in an orthonormal basis, these unitaries form a unitary matrix representation of the abstract group G . Some choices of basis may simultaneously block diagonalize all the unitaries into more than one block. In a basis which maximally block diagonalizes the unitaries, each block carries an irreducible representation (irrep) of G . This basis is unique up to reordering of complete blocks, arbitrary basis transformations within blocks, and recombinations of multiple blocks which carry the same irrep.

Note that: $\hat{U}\hat{H} = \hat{H}\hat{U}$ and $\hat{H}|E\rangle = E|E\rangle$ imply $\hat{H}(\hat{U}|E\rangle) = E(\hat{U}|E\rangle)$. Therefore unitaries in G are block diagonal in any energy basis (with eigenstates sorted by energy). Any further block diagonalization can occur only through basis changes which preserve energy subspaces, therefore there exists an energy basis which maximally block diagonalizes every unitary in $\{\hat{U}_1, \hat{U}_2, \dots\}$. This implies that in the special case in which there is at most one copy of each irrep in the maximal block diagonalization, then any basis which maximally block-diagonalizes the unitaries is an energy basis.

S2. EIGENSTATES AND ENERGIES OF THE HAMILTONIAN

Define $\hat{U}(\hat{V}, \sigma)$ which permutes occupied orbitals by $\sigma \in S_n$ and implements the spin rotation $\hat{V} \in SU(N)$:

$$\hat{U}(\hat{V}, \sigma) |p_1\rangle|p_2\rangle\dots|p_n\rangle \equiv \hat{V}|p_{\sigma^{-1}(1)}\rangle\hat{V}|p_{\sigma^{-1}(2)}\rangle\dots\hat{V}|p_{\sigma^{-1}(n)}\rangle. \quad (\text{S1})$$

These unitaries (for all $\hat{V} \in SU(N)$ and $\sigma \in S_n$) form a well-understood representation of the group $G = SU(N) \times S_n$. Each such unitary commutes with $\hat{H} = \sum_{j \neq k} \hat{s}_{jk}$, where for clarity we dropped all constants from Eq. (1). Irreps of $SU(N)$ and S_n are uniquely labeled by Young diagrams $\vec{\mu}$ and $\vec{\nu}$, respectively, which satisfy different conditions: $\vec{\mu} = (\mu_1, \mu_2, \dots, \mu_N)$, whereas $\sum_i \nu_i = n$. Each irrep of the product group $G = SU(N) \times S_n$ is the tensor product of an irrep of $SU(N)$ and an irrep of S_n and is therefore uniquely labeled by a pair $(\vec{\mu}, \vec{\nu})$. A consequence of Schur-Weyl duality is that representation (S1) block-diagonalizes into exactly one copy of each irrep of G satisfying $\vec{\mu} = \vec{\nu}$, and no other irreps [S1, S2]. Therefore for each Young diagram $\vec{\lambda} = (\lambda_1, \lambda_2, \dots, \lambda_N)$ such that $\sum_i \lambda_i = n$, there is a subspace of constant energy $E(\vec{\lambda})$. One can form an unnormalized projection operator $\hat{\Pi}_{L(\vec{\lambda})}$ into the $\vec{\lambda}$ subspace [S2]:

$$\hat{\Pi}_{L(\vec{\lambda})} = \sum_{\substack{c \in \text{col}(T) \\ r \in \text{row}(T)}} \text{sgn}(c) \hat{U}(\hat{I}, c) \hat{U}(\hat{I}, r). \quad (\text{S2})$$

Here, $L(\vec{\lambda})$ is the labeling of boxes in the Young diagram $\vec{\lambda}$ from 1 to n as shown in Fig. 2(b) in the main text, and $\text{row}(L)$ ($\text{col}(L)$) is the group of all permutations of the numbers 1 to n that preserve the contents of rows (columns) of

$L(\vec{\lambda})$. Applying $\hat{\Pi}_{L(\vec{\lambda})}$ to any state that it does not annihilate returns an eigenstate of energy $E(\vec{\lambda})$. For concreteness we use $|T\rangle \equiv |1, 2, \dots, \gamma_1\rangle |1, 2, \dots, \gamma_2\rangle \dots |1, 2, \dots, \gamma_{\lambda_1}\rangle$, where we also define $\vec{\gamma} = (\gamma_1, \gamma_2, \dots, \gamma_{\lambda_1})$ as the column heights of the Young diagram $\vec{\lambda}$. For each $\vec{\lambda}$ we obtain an explicit eigenstate: $|\vec{\lambda}\rangle = \hat{\Pi}_{L(\vec{\lambda})}|T\rangle$ as in Eq. (2) of the main text. Now we describe how to obtain the eigenvalue $E(\vec{\lambda})$ such that:

$$\hat{H}|\vec{\lambda}\rangle = E(\vec{\lambda})|\vec{\lambda}\rangle. \quad (\text{S3})$$

Premultiplying by $\langle T|$ we obtain: $E(\vec{\lambda}) = \langle T|\hat{H}|\vec{\lambda}\rangle = \sum_{j \neq k} \langle T|\hat{s}_{jk}|\vec{\lambda}\rangle$, noting that $\langle T|\vec{\lambda}\rangle = 1$. For j, k in the same column of the labeled Young diagram $L(\vec{\lambda})$, we know that $\hat{s}_{jk}|\vec{\lambda}\rangle = -|\vec{\lambda}\rangle$. Similarly for j, k in the same row of $L(\vec{\lambda})$ we have $\langle T|\hat{s}_{jk} = \langle T|$. Thus pairs (j, k) in columns contribute -1 to $E(\vec{\lambda})$ and pairs (j, k) in rows contribute $+1$. The number of such pairs can be counted, hence:

$$E(\vec{\lambda}) = \sum_{i=1}^N \binom{\lambda_i}{2} - \sum_{j=1}^{\lambda_1} \binom{\gamma_j}{2} + \sum_{\{j \neq k\}_{\text{diagonal}}} \langle T|\hat{s}_{jk}|\vec{\lambda}\rangle, \quad (\text{S4})$$

The swap \hat{s}_{jk} , where j and k are neither in same column nor in same row in $L(\vec{\lambda})$, can always be written as $\hat{s}_{jk} = \hat{s}_{jm}\hat{s}_{km}\hat{s}_{jm} = \hat{s}_{km}\hat{s}_{jm}\hat{s}_{km}$, where m is chosen such that (j, m) and (k, m) lie in a row and a column of $L(\vec{\lambda})$, respectively (it suffices to consider the case $j > k$). Therefore, $\langle T|\hat{s}_{jk}|\vec{\lambda}\rangle = \langle T|\hat{s}_{km}\hat{s}_{jm}|\vec{\lambda}\rangle = -\langle T|\hat{s}_{km}\hat{s}_{jm}|\vec{\lambda}\rangle = 0$, implying $E(\vec{\lambda}) = \sum_{i=1}^N \binom{\lambda_i}{2} - \sum_{j=1}^{\lambda_1} \binom{\gamma_j}{2}$.

The dimensions of each block can be calculated using the standard hook-length formulae [S3] for any given Young diagram $\vec{\lambda}$. In particular, the ground-state spaces for $U > 0$ and $U < 0$ are $\vec{\lambda}_F = (n, 0, 0, \dots, 0)$ and $\vec{\lambda}_{AF} = (n/N, n/N, \dots, n/N)$ and have dimensions D_F and D_{AF} , respectively:

$$D_F = \frac{(n + N - 1)!}{n! (N - 1)!}, \quad D_{AF} = \frac{n!}{[(n/N)!]^N} \prod_{i=1}^{N-1} \frac{i!}{[n/N + i]}. \quad (\text{S5})$$

S3. DERIVATION OF SPIN DIFFUSION DYNAMICS

We are concerned with observable $\hat{Q} = \sum_{j=1}^{m_1} |1\rangle_j \langle 1|_j$. In this section, we use the notation that for any operator \hat{A} , $A(t) \equiv \langle \psi(0)|e^{i\hat{H}t}\hat{A}e^{-i\hat{H}t}|\psi(0)\rangle$, where $|\psi(0)\rangle = |1\rangle^{\otimes m_1}|2\rangle^{\otimes m_2} \dots |N\rangle^{\otimes m_N}$. As most readers are assumed to be familiar with spin-1/2 systems, we outline the $N = 2$ case first before covering the general case more abstractly.

For $N = 2$, we can choose the angular momentum (Dicke) basis to span the Hilbert space: $|S, S_z, k\rangle$, which diagonalizes the Hamiltonian: $\hat{H}|S, S_z, k\rangle = -US(S+1)|S, S_z, k\rangle$ (dropping a constant energy). The initial state is $|\psi(0)\rangle = |\uparrow\rangle^{\otimes m} |\downarrow\rangle^{\otimes n-m}$ where we used $|\uparrow\rangle$ and $|\downarrow\rangle$ in place of $|1\rangle$ and $|2\rangle$. This state can be understood as a tensor product of two Dicke states on subsets of spins: $|\psi(0)\rangle = |m/2, m/2\rangle \otimes |(n-m)/2, -(n-m)/2\rangle$, where there is no need for a k quantum number since states with $|S_z| = S$ have no additional degeneracy. The tensor product of two angular momentum states can be written as a sum of ‘‘total’’ angular momentum states: $|\psi(0)\rangle = \sum_S C(S)|S, S_z = m - n/2, \alpha(S)\rangle$, where $C(S)$ is a Clebsch-Gordan coefficient, and $\alpha(S)$ represents the fact that $|S, S_z = m - n/2, \alpha(S)\rangle$ is some specific linear combination of Dicke states with the same S and S_z , but different k 's. Hence, $Q(t) = \sum_{S, S'} C(S')^* C(S) e^{iUt[S(S+1) - S'(S'+1)]} \langle S', S_z, \alpha(S')|\hat{Q}|S, S_z, \alpha(S)\rangle$. Note that $\hat{Q} = m\hat{I} + \hat{S}_m^z$ with $\vec{S}_m = \sum_{j=1}^m \vec{S}_j$, and \hat{S}_m^z is the 0-component of the $(S = 1)$ -spherical tensor $\hat{\mathbb{T}} \equiv \{\hat{S}_m^{-1}, \hat{S}_m^z, \hat{S}_m^{+1}\}$, with $\hat{S}_m^{\pm 1} = \mp(\hat{S}_m^x \pm i\hat{S}_m^y)/\sqrt{2}$. We first apply the Wigner-Eckart theorem to write the matrix element in terms of the reduced matrix element and a Clebsch-Gordan coefficient. Then, since $\hat{\mathbb{T}} \equiv \hat{\mathbb{T}}_m \otimes \hat{I}$ acts only on the first m spins, we rewrite [S4, S5] the reduced matrix element on the full system in terms of one on the first m spins and a recoupling coefficient:

$$\langle S', S'_z, \alpha(S')|\hat{Q}|S, S_z, \alpha(S)\rangle = m\delta_{S, S'} + \langle m/2||\hat{\mathbb{T}}_L||m/2\rangle \left\{ \begin{matrix} 1 & m/2 & m/2 \\ (n-m)/2 & S' & S \end{matrix} \right\} (\langle 1, 0| \otimes \langle S, S_z|) |S', S'_z\rangle (\text{S6})$$

where $(\langle 1, 0| \otimes \langle S, S_z|) |S', S'_z\rangle$ is a Clebsch-Gordan coefficient and $\langle m/2||\hat{\mathbb{T}}_L||m/2\rangle$ is the reduced matrix element of $\hat{\mathbb{T}}_L$ on the $S = m/2$ state of the first m spins. The recoupling coefficient $\left\{ \begin{matrix} S_A & S_B & S_{AB} \\ S_C & S & S_{BC} \end{matrix} \right\} \equiv \langle S, S_z, (S_{AB}, S_C)|S, S_z, (S_A, S_{BC})\rangle$ is the overlap between two states of given S and S_z formed from the tensor product

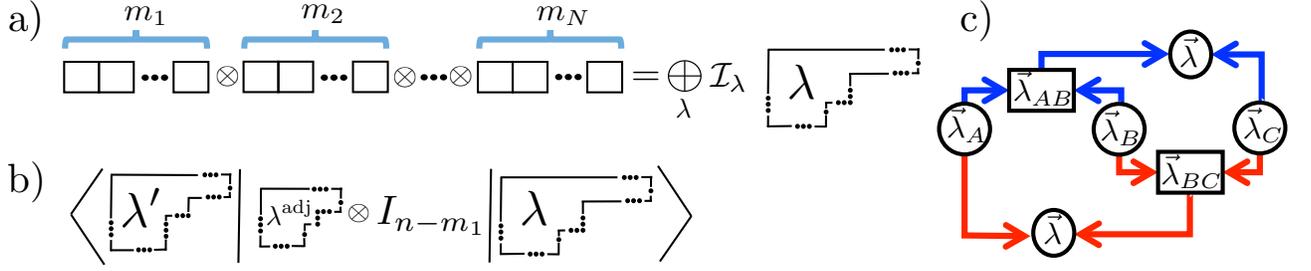


FIG. S1: (a) Initial state $|\psi(0)\rangle$ can be written in terms of energy eigenstates: $|\psi(0)\rangle = |11\dots1\rangle|22\dots2\rangle\dots|NN\dots N\rangle = \sum_{\lambda,a,\alpha} C(\lambda,a,\alpha)|\lambda,a,\alpha\rangle$. (b) Key simplifications arise in the matrix element $\langle\lambda',a',\alpha|Q|\lambda,a,\alpha\rangle$ (which is used to calculate $Q(t)$) since: \hat{Q} is a component of a “spherical tensor” for $SU(N)$ (allowing us to make use of the Wigner-Eckart theorem) and has support only on the first m_1 sites. (c) The recoupling coefficient is defined by taking the direct product of three irreps A , B and C , and finding the overlap between two copies of the same irrep found in two ways: by combining A and B first (top), and by combining B and C first (bottom).

of three subsystems with S_A , S_B and S_C in two different ways: by combining A and B to form S_{AB} first, and by combining B and C to form S_{BC} first. Substitution of the Clebsch-Gordan and recoupling coefficients into the matrix element gives Eq. (4) in the main text.

Now we proceed with the calculation for arbitrary N , simplifying our notation by dropping hats and vectors. The initial state [see Fig. S1(a)] can be written as a direct product of spin-symmetric states $|\psi(0)\rangle = \otimes_{j=1}^{m_1} |1\rangle \otimes_{j=1}^{m_2} |2\rangle \dots \otimes_{j=1}^{m_N} |N\rangle = |\kappa_1, a_1\rangle |\kappa_2, a_2\rangle \dots |\kappa_N, a_N\rangle$, where a_i labels the particular state in the $\kappa_i \equiv (m_i, 0, \dots, 0)$ irrep which corresponds to $|i\rangle^{\otimes m_i}$. The product of $\kappa = (m, 0, \dots, 0)$ with any irrep λ' has no multiplicity [S1]: $|\kappa, a\rangle |\lambda', a'\rangle = \sum_{\lambda'', a''} C(\lambda'', a'') |\lambda'', a''\rangle$, where each irrep λ'' appears at most once and $C(\lambda'', a'') \equiv \langle\lambda'', a'' | (\kappa, a) \kappa', a'\rangle$ is a Clebsch-Gordan coefficient. Applying this iteratively, starting from the right, $|\psi(0)\rangle = \sum_{\lambda,a,\alpha} C(\lambda,a,\alpha) |\lambda,a,\alpha\rangle$, where α labels the set of intermediate irreps, $C(\lambda,a,\alpha)$ can be expressed in terms of Clebsch-Gordan coefficients, and $|\lambda,a,\alpha\rangle$ are orthogonal eigenstates: $H|\lambda,a,\alpha\rangle = E(\lambda)|\lambda,a,\alpha\rangle$. Note: $a \in 1, 2, \dots, \dim[\lambda_{SU(N)}]$ labels a basis state within the λ -irrep of $SU(N)$, and each α labels one distinct copy (out of $\dim[\lambda_{S_n}]$ copies) of the λ -irrep of $SU(N)$ in the Hilbert space $\mathcal{H} = (\mathbb{C}_N)^{\otimes n}$ (all copies of irrep λ of $SU(N)$ in \mathcal{H} sit inside a single copy of irrep λ of $S_n \times SU(N)$). Therefore: $Q(t) = \sum_{\lambda,\lambda',a,a',\alpha} C^*(\lambda',a',\alpha) C(\lambda,a,\alpha) e^{i[E(\lambda')-E(\lambda)]t} \langle\lambda',a',\alpha|Q|\lambda,a,\alpha\rangle$, where we set $a' = \alpha$ since Q has support only on the first m_1 spins. We now outline tools to determine the matrix element $\langle\lambda',a',\alpha|Q|\lambda,a,\alpha\rangle$.

The states $|\lambda,a,\alpha\rangle$ transform according to matrix irrep D^λ of $SU(N)$: $V^{\otimes n}|\lambda,a,\alpha\rangle = \sum_{a'} D_{a'a}^\lambda(V)|\lambda,a',\alpha\rangle$. For each N , there is a set of single-spin operators which generate $SU(N)$: $\tau^{\text{adj}} \equiv \{t_1, t_2, \dots, t_{N^2-1}\}$ which transform according to D^{adj} (the *adjoint irrep* λ_{adj}): $V^{\otimes n} t_a V^{\dagger \otimes n} = \sum_{a'} D_{a'a}^{\text{adj}}(V) t_{a'}$. The set $\{t_1, t_2, \dots, t_{N^2-1}, \hat{I}\}$ forms a basis for $N \times N$ Hermitian matrices: therefore, any single-atom spin observable can be written as $\hat{q} = c_0 \hat{I} + \sum_a c_a t_a$ for some real constants c_a . Therefore $\langle\lambda',a',\alpha|Q|\lambda,a,\alpha\rangle = c_0 + \sum_{a'} c_{a'} \langle\lambda',a',\alpha|T_{a'}^{\text{adj}}|\lambda,a,\alpha\rangle$, where $T_a^{\text{adj}} = \sum_{j=1}^{m_1} t_{aj}$ and $Q = \sum_{j=1}^{m_1} |1\rangle_j \langle 1|_j \equiv \sum_{j=1}^{m_1} \hat{q}_j$. We now prove a generalization of Eq. (S6) to determine the matrix element $\langle\lambda',a',\alpha|T_{a'}^{\text{adj}}|\lambda,a,\alpha\rangle$ [see Fig. S1(b)]. We will need the Wigner-Eckart theorem and recoupling coefficients for $SU(N)$:

$$\langle\lambda',a',\alpha'|T_{a'}^{\lambda''}|\lambda,a,\alpha\rangle = \sum_{\mathcal{I}} \langle\langle\lambda',a',\mathcal{I}||\lambda'',a''\rangle\rangle_{\mathcal{I}} \langle\lambda',\alpha'|T^{\lambda''}||\lambda,\alpha\rangle_{\mathcal{I}}, \quad (\text{S7})$$

$$\left\{ \begin{array}{ccc} \lambda_A & \lambda_B & \lambda_{AB} \\ \lambda_C & \lambda & \lambda_{BC} \end{array} \right\}_{\mathcal{I}_{AB}, \mathcal{I}_C; \mathcal{I}_{BC}, \mathcal{I}_A} \equiv \langle\lambda,a,(\lambda_{AB}, \mathcal{I}_{AB}, \mathcal{I}_C)|\lambda,a,(\lambda_{BC}, \mathcal{I}_{BC}, \mathcal{I}_A)\rangle. \quad (\text{S8})$$

Note that multiplicity \mathcal{I} appears in the Wigner Eckart theorem for $N > 2$ [Eq. (S7)], since the tensor product of irreps can include multiple appearances of the same irrep. The recoupling coefficient defined in Eq. (S8) relates two copies of the same irrep λ formed from the tensor product of three irreps: λ_A , λ_B , and λ_C , but combined in different orders [see Fig. S1(c)]. To define notation: λ_A and λ_B are combined to make λ_{AB} , whose different copies are labeled by \mathcal{I}_{AB} , while \mathcal{I}_C labels different copies of λ when λ_{AB} is combined with λ_C .

One can decompose $|\lambda,a,\alpha\rangle = \sum_{a_1, a_2} D(a_1, a_2) |\kappa_1, a_1\rangle |\lambda_2, a_2\rangle$, where λ_2 is specified by α , and $D \equiv$

$(\langle \kappa_1, a_1 | \langle \lambda_2, a_2 \rangle | \lambda, a, \alpha \rangle)$. Substituting into $\langle \lambda', a', \alpha | T_{a''}^{\text{adj}} | \lambda, a, \alpha \rangle$ and applying Eq. (S7) to the first m_1 spins:

$$\begin{aligned} \langle \lambda', a', \alpha | T_{a''}^{\text{adj}} | \lambda, a, \alpha \rangle &= \langle \kappa_1 | | \mathbb{T}^{\text{adj}} | | \kappa_1 \rangle \sum_{a_1, a'_1, a_2} [(\langle \kappa_1, a'_1 | \langle \lambda_2, a_2 \rangle | \lambda', a' \rangle)^* [(\langle \kappa_1, a_1 | \langle \lambda_2, a_2 \rangle | \lambda, a \rangle) [\langle \kappa, a'_1 | (|\lambda^{\text{adj}}, a''\rangle | \kappa_1, a_1) \rangle]] \\ &= \langle \kappa_1 | | \mathbb{T}^{\text{adj}} | | \kappa_1 \rangle \sum_{\mathcal{I}_1} \left\{ \begin{array}{ccc} \lambda^{\text{adj}} & \kappa_1 & \kappa_1 \\ \lambda_2 & \lambda' & \lambda \end{array} \right\}_{\mathcal{I}_1}^* [(\langle \lambda^{\text{adj}}, a'' | \langle \lambda, a \rangle | \lambda', a', \mathcal{I}_1 \rangle)]. \end{aligned} \quad (\text{S9})$$

The second line represents the generalization of Eq. (S6). To derive Eq. (S9), we return to the abstract scenario of three irreps λ_A , λ_B and λ_C used to define recoupling coefficients in Eq. (S8). First write $|\lambda, a, (\lambda_{AB})\rangle$ as a linear combination of $|\lambda, a, (\lambda_{BC}, \mathcal{I}_A)\rangle$ with Eq. (S8) as coefficients in the special case where $\lambda_B = \lambda_{AB} = \kappa$ (allowing us to drop \mathcal{I}_{AB} , \mathcal{I}_C and \mathcal{I}_{BC}). Rewriting states on both sides as the direct product of states in each of the three subsystems, multiplying by $[\langle \lambda'_{BC}, a_{BC} | (|\lambda_B, a_B\rangle | \lambda_C, a_C)\rangle]$, summing over λ'_{BC} , and using orthogonality gives:

$$\begin{aligned} \sum_{a_{AB}, a_B, a_C} [(\langle \lambda_{AB}, a_{AB} | \langle \lambda_C, a_C \rangle | \lambda, a \rangle) [(\langle \lambda_A, a_A | \langle \lambda_B, a_B \rangle | \lambda_{AB}, a_{1AB})] [\langle \lambda_{BC}, a_{BC} | (|\lambda_B, a_B\rangle | \lambda_C, a_C)\rangle]] &= \\ \sum_{\mathcal{I}_A} \left\{ \begin{array}{ccc} \lambda_A & \kappa & \kappa \\ \lambda_C & \lambda & \lambda_{BC} \end{array} \right\}_{\mathcal{I}_A}^* [(\langle \lambda_A, a_A | \langle \lambda_{BC}, a_{BC} \rangle | \lambda, a, \mathcal{I}_A \rangle)]. \end{aligned} \quad (\text{S10})$$

Using Eq. (S9), the time evolution $T_a(t) \equiv \langle \psi(0) | \exp(iHt) T_a \exp(-iHt) | \psi(0) \rangle$, and therefore $Q(t)$, is written as an efficiently computable sum (containing $poly(n)$ terms [S6], each calculated in $poly(n)$ operations):

$$\begin{aligned} T_a(t) &= \langle \kappa_1 | | \mathbb{T}^{\text{adj}} | | \kappa_1 \rangle \sum_{\lambda'_1, a'_1, \lambda_1, a_1; \alpha} C^*(\lambda'_1, a'_1, \alpha) C(\lambda_1, a_1, \alpha) e^{(i[E(\lambda'_1) - E(\lambda_1)]t)} \\ &\quad \times \sum_{\mathcal{I}_1} \left\{ \begin{array}{ccc} \lambda^{\text{adj}} & \kappa_1 & \kappa_1 \\ \lambda_2 & \lambda'_1 & \lambda_1 \end{array} \right\}_{\mathcal{I}_1} [(\langle \lambda'_1, a'_1, \mathcal{I}_1 | (|\lambda^{\text{adj}}, j\rangle | \lambda_1, a_1) \rangle)]. \end{aligned} \quad (\text{S11})$$

The group-theoretic method presented in this Section was crucial for obtaining the analytical result for $SU(2)$ [Eq. (4) in the main text]. It is also crucial for doing numerics for $SU(N > 2)$ for large n . However, for sufficiently small n , such as the one shown in Fig. 3, one can do the $SU(N > 2)$ numerics using the following simpler method. One first constructs a complete basis of fully symmetric states for the first m_1 spins, for the next m_2 spins, for the next m_3 spins, etc... Then one combines them into a basis for the full system and keeps only those states that have m_1 1's, m_2 2's, m_3 3's, etc... It is straightforward to evaluate the Hamiltonian in this reduced basis and then numerically exponentiate it to calculate time evolution.

S4. HAMILTONIAN DERIVATION: ATOMS WITH CONTACT INTERACTIONS

Contact interactions between two identical multi-component fermionic (bosonic) atoms are described by the Hamiltonian

$$\hat{H}_{int}^{12} = 4\pi\hbar\omega_{\perp} \delta(x_1 - x_2) \otimes \hat{A}, \quad (\text{S12})$$

where the operator \hat{A} only has a physical effect on exchange antisymmetric (symmetric) two-particle internal states because exchange symmetric (antisymmetric) spatial states do not interact. In second quantized form, where \hat{c}_{jr}^{\dagger} creates an atom in internal state r and orbital $\phi_j(x)$ with non-interacting energy E_j , and $W_{k'j'jk} = (4\pi\hbar\omega_{\perp}) \int_0^L dx \phi_{k'}(x)\phi_{j'}(x)\phi_j(x)\phi_k(x)$. The interaction becomes: $\hat{H}_{int} = \sum_{j', k', j, k} W_{k'j'jk} \sum_{r', s', r, s} \langle s', r' | \hat{A} | r, s \rangle \hat{c}_{j'r'}^{\dagger} \hat{c}_{k's'}^{\dagger} \hat{c}_{jr} \hat{c}_{ks}$. Specializing to the infinite square well of width L , to first order in the interaction, only terms satisfying $(j', k') = (j, k)$ or $(j', k') = (k, j)$ survive. Additionally assuming no multiple occupancies, we obtain $W_{kjjk} = W_{jkjk} = W \equiv (4\pi\hbar\omega_{\perp})/L$ for $j \neq k$, and the Hamiltonian becomes:

$$\hat{H} = \sum_{j,r} E_j \hat{c}_{jr}^{\dagger} \hat{c}_{jr} + W \sum_{j,k} \sum_{r', s', r, s} \langle s', r' | \hat{A} | r, s \rangle \left(\hat{c}_{j'r'}^{\dagger} \hat{c}_{k's'}^{\dagger} \hat{c}_{jr} \hat{c}_{ks} + \hat{c}_{k'r'}^{\dagger} \hat{c}_{j's'}^{\dagger} \hat{c}_{jr} \hat{c}_{ks} \right). \quad (\text{S13})$$

For the special case of (fermionic) alkaline-earth atoms, \hat{A} cannot depend on nuclear spin; therefore $\hat{A} = (a_{ee}|e, e\rangle\langle e, e| + a_{gg}|g, g\rangle\langle g, g| + a_{eg}^+|e, g\rangle\langle e, g|_+ + a_{eg}^-|e, g\rangle\langle e, g|_- - \langle e, g|_-) \otimes \hat{I}_{Nuclear}$, where $|e, g\rangle_{\pm} = (|e, g\rangle \pm |g, e\rangle)/\sqrt{2}$ [S7]. Under these conditions, and applying a strong magnetic field (which to first order in perturbation theory prevents exchanges $|ep, gq\rangle \leftrightarrow |eq, gp\rangle$), we obtain Eq. (5) with $U_{1g2g} = U_{2g1g} = U_{gg} \equiv 4\pi\omega_{\perp} a_{gg}/L$, $U_{1e2e} = U_{2e1e} = U_{ee} \equiv 4\pi\omega_{\perp} a_{ee}/L$, $U_{1g1e} = U_{2g2e} = U_{1g2e} = U_{2g1e} = U_{eg} \equiv 2\pi\omega_{\perp} (a_{eg}^+ + a_{eg}^-)/M$.

S5. GHZ STATE PREPARATION

The state $|A\rangle = |1g1g\dots1g\rangle$ has energy $E_A = nB_g$. The state $|B\rangle = \{|1e1g\dots1g\rangle\}$ lies in the same energy manifold as the state $(|1g1e\rangle - |1e1g\rangle)|1g\dots1g\rangle$, which has energy $E_B = \omega_{eg} + (n-1)B_g + B_e + [(n-1) - (-1)]U_{1g1e}$. Similarly, $|C\rangle = \{|1e1e\dots1g\rangle\}$ has the same energy as $(|1g1e\rangle - |1e1g\rangle)(|1g1e\rangle - |1e1g\rangle)|1g\dots1g\rangle$, with energy $E_C = 2\omega_{eg} + (n-2)B_g + 2B_e + [2(n-2) - (-2)]U_{1g1e}$. Driving with frequency $(E_B - E_A)$ forms an effective two-level system: $\{|A\rangle \leftrightarrow |B\rangle \nleftrightarrow |C\rangle\}$ since $(E_B - E_A) = \omega_{eg} - B_g + B_e + nU_{1g1e} \neq (E_C - E_B) = \omega_{eg} - B_g + B_e + (n-2)U_{1g1e}$.

Now we explain why transition $|A\rangle \rightarrow |D\rangle \equiv |2g2g\dots2g\rangle$ occurs, while the transition $|B\rangle \nleftrightarrow |x\rangle$ is blocked for any energy eigenstate $|x\rangle$. First note that the transition $|A\rangle \rightarrow |D\rangle$ actually passes through a ladder of intermediate energy eigenstates: $|A\rangle \equiv |1g1g\dots1g\rangle \rightarrow |\mathcal{S}\{2g1g\dots1g\}\rangle \rightarrow |\mathcal{S}\{2g2g\dots1g\}\rangle \rightarrow \dots \rightarrow |2g2g\dots2g\rangle \equiv |D\rangle$, where \mathcal{S} symmetrizes its argument. Each state in the ladder has energy $2B_g$ more than the last, and is connected to the previous through the operator $\hat{P} = \sum_j (|2g\rangle_j \langle 1g|_j + |2e\rangle_j \langle 1e|_j)$, which is applied as a pulse with frequency $2B_g$. To show that $|B\rangle$ does not transition to any other state under the action of this pulse, we must prove that *there exists no state $|x\rangle$ such that $\hat{H}|x\rangle = (E_B + 2B_g)|x\rangle$ and $\langle x|\hat{P}|B\rangle \neq 0$* . We will assume that $n > 2$, $B_e \neq B_g$ and either $|U_{gg}| > 0$ or $|U_{eg}| > 0$.

Our proof has the following structure: we find four orthonormal states such that $\hat{P}|B\rangle \in \text{span}\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle\} \equiv \mathcal{H}_0$, where subspace \mathcal{H}_0 is closed under the action of \hat{H} (i.e. for all $|\psi\rangle \in \mathcal{H}_0$, $\hat{H}|\psi\rangle \in \mathcal{H}_0$). Any eigenstate $|x\rangle$ of \hat{H} coupled to $|B\rangle$ through \hat{P} must be in \mathcal{H}_0 , but we show the four eigenvalues E_i of \hat{H} in \mathcal{H}_0 satisfy $E_i \neq (E_B + 2B_g)$.

To complete the proof, we must present $\{|\phi_1\rangle, |\phi_2\rangle, |\phi_3\rangle, |\phi_4\rangle\}$ explicitly, and show that $E_i \neq (E_B + 2B_g)$ for all four eigenstates ($i = 1, 2, 3, 4$). Without loss of generality, take $|B\rangle = (|1g1e\rangle - |1e1g\rangle)|1g\dots1g\rangle$, thus $\hat{P}|B\rangle = \sqrt{2(n-2)}|\phi_1\rangle + \sqrt{2}|\phi_3\rangle + \sqrt{2}|\phi_4\rangle$, where $|\phi_1\rangle \equiv \frac{1}{\sqrt{2(n-2)}}(|1g1e\rangle - |1e1g\rangle)|\mathcal{S}\{1g2g\dots1g\}\rangle$, $|\phi_2\rangle \equiv \frac{1}{\sqrt{2}}(|2g1e\rangle - |1e2g\rangle)|1g1g\dots1g\rangle$, $|\phi_3\rangle \equiv \frac{1}{\sqrt{2(n-2)}}(|1g2g\rangle - |2g1g\rangle)|\mathcal{S}\{1g1e\dots1g\}\rangle$, and $|\phi_4\rangle \equiv \frac{1}{\sqrt{2}}(|1g2e\rangle - |2e1g\rangle)|1g1g\dots1g\rangle$ (note that $|\phi_4\rangle$ is an energy eigenstate). \hat{H} is closed on subspace \mathcal{H}_0 and takes the form:

$$\hat{H} = (E_B + 2B_g) + \begin{pmatrix} 0 & -\sqrt{n-2}U_{gg} & -U_{ge} & 0 \\ -\sqrt{n-2}U_{gg} & (n-2)U_{gg} & \sqrt{n-2}U_{ge} & 0 \\ -U_{ge} & \sqrt{n-2}U_{ge} & (n-1)U_{gg} - U_{ge} & 0 \\ 0 & 0 & 0 & 2(B_g - B_e) \end{pmatrix}. \quad (\text{S14})$$

The matrix written explicitly in Eq. (S14) can be shown to have non-zero determinant (and therefore no vanishing eigenvalues) provided $n > 2$, $B_e \neq B_g$ and either $|U_{gg}| > 0$ or $|U_{eg}| > 0$, which completes our proof.

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