Two-orbital SU(N) magnetism with ultracold alkaline-earth atoms

A. V. Gorshkov\textsuperscript{1,*}, M. Hermele\textsuperscript{2}, V. Gurarie\textsuperscript{2}, C. Xu\textsuperscript{1}, P. S. Julienne\textsuperscript{3}, J. Ye\textsuperscript{4}, P. Zoller\textsuperscript{5}, E. Demler\textsuperscript{1,6}, M. D. Lukin\textsuperscript{1,6}, and A. M. Rey\textsuperscript{4}

\textsuperscript{1}Physics Department, Harvard University, Cambridge, MA 02138
\textsuperscript{2}Department of Physics, University of Colorado, Boulder, CO 80309
\textsuperscript{3}Joint Quantum Institute, NIST and University of Maryland, Gaithersburg, MD 20899-8423
\textsuperscript{4}JILA, NIST, and Department of Physics, University of Colorado, Boulder, CO 80309
\textsuperscript{5}Institute for Theoretical Physics, University of Innsbruck, A-6020 Innsbruck, Austria and Institute for Quantum Optics and Quantum Information of the Austrian Academy of Sciences, A-6020 Innsbruck, Austria
\textsuperscript{6}Institute for Theoretical Atomic, Molecular and Optical Physics, Harvard-Smithsonian Center of Astrophysics, Cambridge, MA 02138 and
\textsuperscript{*}e-mail: gorshkov@post.harvard.edu

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Fermionic alkaline-earth atoms have unique properties that make them attractive candidates for the realization of novel atomic clocks and degenerate quantum gases. At the same time, they are attracting considerable theoretical attention in the context of quantum information processing. Here we demonstrate that when such atoms are loaded in optical lattices, they can be used as quantum simulators of unique many-body phenomena. In particular, we show that the decoupling of the nuclear spin from the electronic angular momentum can be used to implement many-body systems with an unprecedented degree of symmetry, characterized by the SU(N) group with N as large as 10. Moreover, the interplay of this nuclear spin with the electronic degree of freedom provided by a stable optically excited state allows for the study of spin-orbital physics. Such systems may provide valuable insights into strongly correlated physics of transition metal oxides, heavy fermion materials, and spin liquid phases.

The interest in fermionic alkaline-earth atoms stems from their two key features: (1) the presence of a metastable excited state coupled to the ground state via an ultranarrow doubly-forbidden transition and (2) the almost perfect decoupling of the nuclear spin from the electronic angular momentum. This decoupling implies that s-wave scattering lengths involving states and are independent of the nuclear spin, aside from the restrictions imposed by fermionic antisymmetry. We show that the resulting SU(N) spin symmetry (where ) can be as large as 10) together with the possibility of combining (nuclear) spin physics with (electronic) orbital physics open up a wide field of extremely rich many-body systems with alkaline-earth atoms.

In what follows, we derive the two-orbital SU(N)-symmetric Hubbard model describing alkaline-earth atoms trapped in an optical lattice. We focus on specific parameter regimes characterized by full or partial atom localization due to strong atomic interactions, where simpler effective spin Hamiltonians can be derived. The interplay between orbital and spin degrees of freedom in such effective models is a central topic in quantum magnetism and has attracted tremendous interest in the condensed matter community. Alkaline earth atoms thus provide, on the one hand, a unique opportunity for the implementation of some of these models for the first time in a defect-free and fully controllable environment. On the other hand, they open a new arena to study a wide range of models, many of which have not been discussed previously, even theoretically. We demonstrate, in particular, how to implement the Kugel-Khomskii model studied in the context of transition metal oxides, the Kondo lattice model, the symmetric Hubbard model describing alkaline-earth atoms, and the many-body systems with alkaline-earth-like atoms make a truly exceptional system to study models with SU(N=2) symmetry.

manganese oxide perovskites and heavy fermion materials, as well as various SU(N)-symmetric spin Hamiltonians that are believed to have spin liquid and valence-bond solid ground states. For example, we discuss how, by appropriately choosing the initial state, a single alkaline-earth atom species with can be used to study experimentally such a distinctively theoretical object as the phase diagram as a function of N for all .

Before proceeding, we note that, while an orthogonal symmetry group SO(5) can be realized in alkali atoms, proposals to obtain SU(N>2)-symmetric models with alkali atoms and solid state systems are a substantial idealization due to strong hyperfine coupling and a complex solid state environment, respectively. In this context, alkaline-earth-like atoms make a truly exceptional system to study models with SU(N=2) symmetry.
Many-body dynamics of alkaline-earth atoms in an optical lattice

We begin with the Hamiltonian describing cold fermionic alkaline-earth atoms in an external trapping potential:

\[
H = \sum_{\alpha m} \int d^3 r \Psi^\dagger_{\alpha m}(r)(-\frac{\hbar^2}{2M} \nabla^2 + V_\alpha(r))\Psi_{\alpha m}(r)
\]

\[
+ \hbar \omega_0 \int d^3 r (\rho_\alpha(r) - \rho_\gamma(r)) + \frac{g_{eg}^+ + g_{eg}^-}{2} \int d^3 r \rho_\gamma(r)\rho_\gamma(r)
\]

\[
+ \sum_{\alpha, m < m'} g_{\alpha m} \int d^3 r \rho_{\alpha m}(r)\rho_{\alpha m'}(r)
\]

\[
+ \frac{g_{eg}^+ - g_{eg}^-}{2} \sum_{mm'} \int d^3 r \Psi^\dagger_{g m}(r)\Psi_{g m'}(r)\Psi_{e m'}(r)\Psi_{e m}(r).
\]

Here \(\Psi_{\alpha m}(r)\) is a fermion field operator for atoms in internal state \(|\alpha m\rangle\), where \(\alpha = g(1S_0)\) or \(e (2P_0)\) denotes the electronic state and \(m = -I, \ldots, I\) denotes one of the \(N = 2I+1\) nuclear Zeeman states. The density operators are defined as \(\rho_{\alpha m}(r) = \Psi^\dagger_{\alpha m}(r)\Psi_{\alpha m}(r)\) and \(\rho_\gamma(r) = \sum_{\alpha m} \rho_{\alpha m}(r)\). The term \(V_\alpha(r)\) describes the external trapping potential, which we will assume to be an optical lattice independent of the nuclear spin: even for a relatively deep lattice with a 100 kHz trap frequency, tensor and vector light shifts should be well below 1 Hz [1]. \(\hbar \omega_0\) is the transition energy between \(|g\rangle\) and \(|e\rangle\). Extra lasers can be used to drive transitions between \(|g\rangle\) and \(|e\rangle\) levels [1, 2]. Since we will only need these extra lasers for system preparation, we have not included the corresponding terms in the Hamiltonian.

The interaction is characterized by four s-wave scattering lengths \(a_X\), \(X = gg, ee, eg^+, eg^-\), which define four interaction parameters \(g_X = 4\pi\hbar^2 a_X/M\), where \(M\) is atomic mass. \(a_{gg}, a_{ee}\), and \(a_{eg}^\pm\) are the scattering length for two atoms in the electronic state \(|gg\rangle\), \(|ee\rangle\), and \(|\pm\rangle = (|gg\rangle + |eg\rangle)/\sqrt{2}\), respectively. As shown in Fig. 1 the fermionic antisymmetry then forces the nuclear state to be symmetric for the only antisymmetric electronic state \(|-\rangle\) and antisymmetric otherwise. Very few \(a_X\) are known at the moment (see Supplementary Information).

The independence of each of the four scattering lengths from the nuclear spin state is essential to the fulfillment of the SU(N) symmetry of our model (see next Section). This independence is a consequence of the decoupling between nuclear and electronic degrees of freedom exhibited during the course of a collision involving any combination of \(g\) or \(e\) states, which both have \(J = 0\). While for the \(|e\rangle \equiv 2P_0\) atom, the decoupling is slightly broken by the admixture with higher-lying \(P\) states with \(J \neq 0\), this admixture is very small [1] and the resulting nuclear-spin-dependent variation of the scattering lengths is also expected to be very small, on the order of \(10^{-3}\) (see Supplementary Information). For \(a_{gg}\), which does not involve state \(|e\rangle\), this variation should be even smaller (~\(10^{-9}\)).

The interaction terms in Eq. (1) describe the most general s-wave two-body interaction consistent with elastic collisions as far as the electronic state is concerned and with the independence of the scattering length from the nuclear spin. While the assumption of elasticity for \(g\)-\(g\) and \(e\)-\(g\) collisions is well justified, since no inelastic exit channels exist, \(e\)-\(e\) collisions are likely to be accompanied by large losses, which means that the magnitudes of the imaginary and real parts of the \(e\)-\(e\) scattering length are likely to be comparable (see Supplementary Information). Therefore, we focus below on those situations where two \(e\) atoms never occupy the same site.

We assume that only the lowest band in both \(e\) and \(g\) lattices is occupied and expand the field operators in terms of the corresponding (real) Wannier basis functions \(\Psi_{\alpha m}(r) = \sum_j w_{\alpha j}(r - r_j)\psi_{Jam}\), where \(c^\dagger_{Jam}\) creates an atom in internal state \(|\alpha m\rangle\) at site \(j\) (centered at position \(r_j\)). Eq. (1) reduces then to a two-orbital single-band Hubbard Hamiltonian

\[
H = -\sum_{\langle j, i \rangle \alpha m} J_{\alpha j}(c^\dagger_{Jam}c_{Jam} + \text{h.c.}) + \sum_{j, \alpha} \frac{U_{\alpha j}}{2} n_{\alpha j}(n_{\alpha j} - 1)
\]

\[
+ V \sum_j n_{je} n_{jg} + V_{ex} \sum_{j, m, m'} c^\dagger_{jgm} c^\dagger_{jem} c_{jgm} c_{jem}.
\]

Here \(J_{\alpha j} = -\int d^3 r w_{\alpha j}(r)(-\frac{\hbar^2}{2M} \nabla^2 + V_{\alpha}(r))w_{\alpha j}(r - r_0)\) are the tunneling energies, \(r_0\) connects two nearest neighbors, h.c. stands for Hermitian conjugate, \(n_{jam} = c^\dagger_{jam}c_{jam}\), and \(n_{ja} = \sum_{m} n_{jam}\). The tunneling is isotropic, which is a crucial difference between this model and its analogues in solid state systems with orbital degeneracy [9]. The sum \(\langle j, i \rangle\) is over pairs of nearest neighbor sites \(i, j\). \(V = (U_{eg}^+ + U_{eg}^-)/2\) and \(V_{ex} = (U_{eg}^+ - U_{eg}^-)/2\) describe the direct and exchange interaction terms. The onsite interaction energies are \(U_{\alpha j} = g_{\alpha j} \int d^3 r w_{\alpha j}^2(r)\) and \(U_{eg}^\pm = g_{eg}^\pm \int d^3 r w_{eg}^2(r)\). Constant terms, proportional to \(\sum_j n_{ja}\), are omitted in Eq. (2). Experimental control over the parameters in Eq. (2) will allow us to manipulate the atoms (see Methods).
Symmetries of the Hamiltonian

To understand the properties of the Hamiltonian in Eq. (2), we consider its symmetries. We define SU(2) pseudo-spin algebra via

$$T^μ = \sum_j T^μ_j = \frac{1}{2} \sum_{j, \alpha, \beta} \epsilon^{\mu \alpha \beta} c^\dagger_{j \alpha} \sigma^\mu_{\alpha \beta} c_{j \beta},$$

where $\sigma^\mu (\mu = x, y, z)$ are Pauli matrices in the $\{e, g\}$ basis. We further define nuclear-spin permutation operators

$$S^m_n = \sum_j S^m_n(j) = \sum_{j, \alpha} S^m_n(j, \alpha) = \sum_{j, \alpha} \epsilon^{1 \alpha \mu} c^\dagger_{j \alpha} c_{j m},$$

which satisfy the SU(N) algebra $[S^m_n, S^p_q] = \delta_{nq} S^p_n - \delta_{ pn} S^m_q$, and thus generate SU(N) rotations of nuclear spins ($N = 2I + 1$).

In addition to the obvious conservation of the total number of atoms $n = \sum_j (n_{je} + n_{jj})$, $H$ exhibits $U(1) \times SU(N)$ symmetry (see Methods for the discussion of enhanced symmetries), where $U(1)$ is associated with the elasticity of collisions as far as the electronic state is concerned ($[T^z, H] = 0$) and SU(N) is associated with the independence of scattering and of the trapping potential from the nuclear spin ($[S^m_n, H] = 0$ for all $n, m$).

The two-orbital SU(N)-symmetric Hubbard Hamiltonian in Eq. (2) is a generalization to $N > 2$ of its SU(2)-symmetric counterpart [9] and to two orbitals of its single-orbital counterpart [28]. The SU(N) symmetry and the largely independent spin and orbital degrees of freedom are two unique features present in alkaline-earths but absent in alkalis due to strong hyperfine interactions.

One important consequence of SU(N) symmetry is the conservation, for any $m$, of $S^m_n$, the total number of atoms with nuclear spin $m$. This means that an atom with large $I$, e.g. $^{87}$Sr ($I = 9/2$), can reproduce the dynamics of atoms with lower $I$ if one takes an initial state with $S^m_m = 0$ for some $m$ values. To verify SU(N) symmetry of the interaction experimentally, one could, thus, put two atoms in one well in spins $m$ and $m'$ and confirm that collisions do not populate other spin levels. This feature of SU(N) symmetry is in stark contrast to the case of weaker SU(2) symmetry, where the dependence of scattering lengths on the total spin of the two colliding particles allows for scattering into spin states other than $m$ and $m'$. We note that although collisions are governed by electronic interactions and obey the nuclear-spin SU(N) symmetry, the nuclear spins still indirectly control the collisions via fermionic statistics and give rise to effective spin-orbital and spin-spin interactions.

One can alternatively implement the two-orbital Hubbard model with two ground-state species of alkaline-earth atoms (e.g. $^{171}$Yb and $^{173}$Yb, or $^{173}$Yb and $^{87}$Sr). If we still refer to them as $|g⟩$ and $|e⟩$, the nuclear distinguishability and the fact that both atoms are in the ground state will result in $a^\dagger_{eg} = a^\dagger_{ge}$, corresponding to an enhanced symmetry (see Methods). While experimentally more challenging, the use of two different ground state species will solve the problem of losses associated with collisions of two excited state atoms and will reduce the (already very weak) nuclear-spin-dependence of $a_{ee}$ and $a_{eg}$.

Spin Hamiltonians

One of the simplest interesting limits of Eq. (2) is the strongly interacting regime ($J/U \ll 1$) where the Hilbert space is restricted to a given energy manifold of the $J_y = J_z = 0$ Hamiltonian (with a fixed number of atoms on each site), and tunneling is allowed only virtually, giving rise to an effective spin (and pseudo-spin) Hamiltonian. Single-site energy manifolds can be classified according to the number of atoms $n_j = n_{gg} + n_{je}$, the pseudo-spin component $T^z$, and the spin symmetry (SU(N) representation) described by a Young diagram. As shown in Fig. 2, each diagram consists of $n_j$ boxes and at most two columns of heights $p$ and $q$, representing two sets of antisymmetrized indices.

The $U(1) \times SU(N)$ symmetry of Eq. (2) restricts the order $J^2$ spin Hamiltonian to the form

$$H_{p,q} = \sum_{(i, j), \alpha} \left[ \kappa_{\alpha \kappa} n_{i \alpha} n_{j \kappa} + \lambda_{\alpha \lambda} S^m_n (i, \alpha) S^m_n (j, \alpha) \right] + \sum_{(i, j)} \left[ \kappa_{ge} n_{i g} n_{j e} + \lambda_{ge} S^m_n (i, g) S^m_n (j, e) \right] + \kappa_{eq} n_{i q} n_{j e} + \lambda_{eq} S^m_n (i, q) S^m_n (j, e) + \{ i \leftrightarrow j \} \right].$$

where the sum over $n$ and $m$ is implied in all but the $κ$ terms and $S^m_n (j) = c^\dagger_{j g} c_{j m}$. $\{ i \leftrightarrow j \}$ means that all 4 preceding terms are repeated with $i$ and $j$ exchanged. The coefficients $κ$, $λ$, $κ$, and $λ$ are of order $J^2/U$ with the exact form determined by what single-site energy manifolds we are considering. $κ$ terms describe nearest neighbor repulsion or attraction, while $λ$, $κ$, and $λ$ terms describe nearest neighbor exchange of spins, pseudo-spins, and complete atomic states, respectively. Without loss of generality, $κ_{\alpha \kappa} = κ_{\alpha \kappa}^{ij}$ and $λ_{\alpha \lambda} = λ_{\alpha \lambda}^{ij}$. In many cases (e.g. case (2) below), the Hilbert space, which $H_{p,q}$
**FIG. 3:** The ground-state phase diagram for the SU(N=2) Kugel-Khomskii model restricted to two wells, left (L) and right (R). 

- **a** $T_z = -1$
- **b** $T_z = 0$

The phase diagram for $T_z = -1$ (two g atoms) and $T_z = 0$ (one g and one e atom) is shown in Fig. 2b. The phase diagram for $T_z = 0$ (one g atom and one e atom) is shown in Fig. 2a. A third case, $(p, q) = (1, 1)$, which reduces for $N = 2$ to the spin-1 Heisenberg antiferromagnet is discussed in the Supplementary Information.

(1) In the case of one atom per site, $(p, q) = (1, 0)$, $H_{(p,q)}$ is then a generalization to arbitrary N of the SU(N = 2) Kugel-Khomskii model [9,13], and we rewrite it as (see Supplementary Information)

$$H_{(1,0)} = \sum_{\langle i,j \rangle} \left[ 2(\tilde{k}_{ge} + \lambda_{ge}S^2_{ij}T^\omega_j) + h \right]$$

where $S^2_{ij} = \sum_{m,n} S^m_g(i)S^n_g(j)$ is $+1$ ($-1$) for a symmetric (antisymmetric) spin state, $A = 2\lambda_{ge} - \kappa_e - \kappa_g$, $B = 2\lambda_{ge} + \kappa_e + \kappa_g$, and $h = (\kappa_e - \kappa_g)/2$. The $N = 2$ Kugel-Khomskii Hamiltonian is used to model the spin-orbital interactions (not to be confused with relativistic spin-orbit coupling) in transition metal oxides with perovskite structure [13]. Our implementation allows to realize clean spin-orbital interactions unaffected by lattice and Jahn-Teller distortions present in solids [13].

To get a sense of the competing spin and orbital orders [10,11,12] characterizing $H_{(1,0)}$, we consider the simplest case of only two sites (L and R) and $N = 2$ (with spin states denoted by $\uparrow$ and $\downarrow$). To avoid losses in $e-e$ collisions, we set $U_{ee} = \infty$ (see Supplementary Information). The double-well ground-state phase diagram for $T^z = 1$ (two e atoms) is then trivial, while the $T^z = -1$ (two g atoms) and $T^z = 0$ (one g atom and one e atom) diagrams are shown in Fig. 3. One can see that, depending on the signs and relative magnitudes of the interactions, various combinations of ferromagnetic (triplet) and antiferromagnetic (singlet) spin and orbital orders are favored. In the Methods, we propose a double-well experiment along the lines of Ref. [39] to probe the spin-orbital interactions giving rise to the $T^z = 0$ diagram in Fig. 3b. Multi-well extensions of this experiment may shed light on the model’s many-body phase diagram, which has been studied for $N = 2$ and mostly at mean-field level or in special cases, such as in one dimension or in the presence of enhanced symmetries (see e.g. [11,12]).

(2) In order to study SU(N) spin physics alone, we consider the case of $g$ atoms only. On a bipartite lattice with sublattices A and B, we choose A sites to have $n_A < N$ atoms and B sites to have $n_B < N$ atoms. This setup can be engineered in cold atoms by using a superlattice to adjust the depths of the two sublattices favoring a higher filling factor in deeper wells. $H_{(p,q)}$ then reduces to

$$H_{(p,0)} = \frac{2J_{gg}^2U_{gg}}{U_{gg}^2 - (U_{gg}(n_A - n_B) + \Delta)^2} \sum_{\langle i,j \rangle} S^2_{ij}$$

where $\Delta$ is the energy offset between adjacent lattice sites. The coupling constant can be made either positive (antiferromagnetic) or negative (ferromagnetic) depending on the choice of parameters [39]. Three body recombination processes will likely limit the lifetime of the atoms when $n_j \geq 3$ (see Supplementary Information).

We focus on the 2D square lattice in the antiferromagnetic regime. The case $n_A + n_B = N$ shares with the SU(2) Heisenberg model the crucial property that two adjacent spins can form an SU(N) singlet, and has thus been studied extensively as a large-N generalization of SU(2) magnetism [27,28]. Fig. 4 shows the expected phase diagram...
for the case \( n_A + n_B = N \), which features Neel (circles), valence-bond-solid (VBS) (squares) [Fig. 4(b)], and possible critical spin liquid (triangle) [30, 31] ground states. To access various ground states of the system, the initial state must be carefully prepared so that the conserved quantities \( S_n^{(m)} \) take values appropriate for these ground states. Another interesting and experimentally relevant case, \( n_A = n_B \neq N/2 \), which can also exhibit spin liquid and VBS-type ground states, is discussed in the Supplementary Information and in Ref. [34].

Since one can vary \( N \) just by choosing the number of initially populated Zeeman levels (e.g. via a combination of optical pumping and coherent manipulation), alkaline-earth atoms offer a unique arena to probe the phase diagram of \( H_{p,0} \), including exotic phases such as VBS [Fig. 4(b)], as well as competing magnetically ordered states. We propose to load a band insulator of \( N \) \( g \) atoms per site, then slowly split each well into two to form an array of independent SU(N) singlets in a pattern shown in Fig. 4(b). The intersinglet tunneling rate should then be adiabatically increased up to the intrasinglet tunneling rate. As \( N \) increases, the magnetic or singlet nature of the state can be probed by measuring the Neel order parameter (see the description of the Kugel-Khomskii double-well experiment in the Methods) and spin-spin correlations via isotope spectroscopy in the time of flight [40] (which directly measures \( \sum_{i,j} \langle S_i^{(m)} (i,g) S_j^{(m)} (j,g) \rangle e^{iQ(i-j)} \)).

The Kondo lattice model (KLM)

The SU(N) Kondo lattice model (KLM) [15, 17] is another example of the rich physics, beyond the Mott regime, which could be simulated with alkaline-earth atoms. The KLM is one of the canonical models used to study strongly correlated electron systems, such as manganese oxide perovskites [20] and rare earth and actinide compounds classed as heavy fermion materials [25].

For its implementation with cold atoms (for \( N = 2 \), see also Refs. [23, 24]), we propose to put one \( e \) atom (localized spin) per site in a deep lattice such that \( J_e \ll U_{ee} \), so that we can set \( J_e = 0 \) and \( n_{je} = 1 \) for all \( j \) in Eq. (2). We also suppose that we can set \( U_{gg} = 0 \), e.g. by taking a very shallow \( g \)-lattice (see Fig. 5a). The resulting Hamiltonian is the SU(N) KLM [15, 17]

\[
H_{KLM} = -\sum_{\langle i,j \rangle, m} J_g (c_{igm}^+ c_{jgm} + h.c.) + \sum_{j,m,m'} V_{ex} c_{jgm}^+ c_{jm'} c_{jgm'} c_{jpm'}
\]

The magnitude of \( V_{ex} \) can be adjusted by shifting the \( e \) and \( g \) lattices relative to each other [17].

The properties of the SU(N) KLM depend crucially on the sign of the exchange interaction. For concreteness, we focus on the antiferromagnetic (AF) case (\( V_{ex} < 0 \)), which favors formation of spin-antisymmetric states (singlets, for \( N = 2 \)) between mobile fermions and localized spins. This regime describes the physics of heavy fermion materials [25], and, in the case of a single localized spin, gives rise to the Kondo effect.

In the limit \( |V_{ex}| \ll J_g \), \( g \) atoms mediate long-range RKKY interactions [14] between localized spins and tend to induce magnetic ordering (antiferromagnetic or ferromagnetic depending on the density of \( g \) atoms) of the latter, at least for \( N = 2 \). The engineering of RKKY interactions can be tested in an array of isolated double wells (see Methods). At intermediate and large \( |V_{ex}| \), the formation of Kondo singlets dominates the RKKY interaction and favors a magnetically disordered heavy Fermi liquid (HFL) ground state with a sig-

\[ T_{RKKY} \]

AF

HFL

FIG. 5: Kondo lattice model for the case \( N = 2 \). a. The schematic of the setup. \( g \) atoms are green; \( e \) atoms are yellow; the spin basis is \{↑, ↓\}. b. Schematic representation of the competition between RKKY magnetism vs Kondo singlet formation in the SU(2) AF KLM (see [16, 26, 28] and references therein). In this model, the localized spin-1/2 \( e \) atoms couple antiferromagnetically to the \( g \) delocalized \( g \) atoms, via an on-site exchange interaction proportional to \( V_{ex} \). This coupling favors the formation of localized Kondo singlets between \( e \) and \( g \) atoms, with characteristic energy scale \( k_B T_K \approx J_g \exp (-c J_g / |V_{ex}|) \), with \( c \) a dimensionless constant of order one [25]. On the other hand, the \( g \) atoms can mediate long-range RKKY interactions between the \( e \) atoms, giving rise to magnetic order (which can be antiferromagnetic (AF) or ferromagnetic depending on the density of \( g \) atoms), where the characteristic energy is \( k_B T_{RKKY} \approx V_{ex} / J_g \). The competition between Kondo effect and RKKY magnetism leads to very rich physics. For small values of \( |V_{ex}| / J_g \), the RKKY interaction is dominant and the system orders magnetically. At intermediate values of \( |V_{ex}| / J_g \), the energy scales \( T_K \) and \( T_{RKKY} \) are of comparable strength, and a variety of novel quantum phenomena are expected to arise, including quantum criticality and non-Fermi liquid (NFL) physics [25, 26]. With further increase of the \( |V_{ex}| / J_g \) coupling, magnetic order is suppressed, the localized \( e \) atoms become screened into singlet states and melt into the \( g \)-atom Fermi sea, forming the so called heavy Fermi liquid state (HFL). The large Fermi volume [26], which is set by the total number of \( g \) atoms plus \( e \) atoms, can be directly probed by measuring the momentum distribution via time of flight imaging.
significantly enhanced effective quasiparticle mass (see Fig. 5). The competition between RKKY interactions and the Kondo effect in the regime where both are comparable is subtle, and the resulting phases and phase transitions [25, 26] are not well-understood. Ultracold alkaline-earth atoms provide a promising platform to study these phases and phase transitions.

In the large-$N$ limit [15, 17], the SU(N) HFL can be controllably studied, and $1/N$ expansions have successfully reproduced the experimentally observed properties of the HFL. However, very little is known about the SU(N) model outside the HFL regime. Several very interesting parameter regimes in this domain can be directly probed with our system, as discussed in the Methods.

Experimental Accessibility

The phenomena described in this manuscript can be probed with experimental systems under development. Indeed, we show in the Methods that SU(N)-breaking terms are sufficiently weak, and here we discuss the temperature requirements.

The key energy scale in the spin Hamiltonians [Eq. (5)] is the superexchange energy $J^2/U$, while the RKKY energy scale is $k_BT_{RKKY} \sim V_{ex}^2/J_g$. In their region of validity ($J < U$ and $|V_{ex}| < J_g$, respectively), these energy scales are limited from above by the interaction energy ($U$ and $|V_{ex}|$, respectively), which typically corresponds to temperatures $T \lesssim 100\text{nK}$ [39]. Thanks to the additional cooling associated with certain adiabatic changes [41, 42], $T \sim 10\text{nK}$ and the Mott insulating regime have already been achieved with fermionic alkaline atoms [43], and are therefore expected to be achievable with fermionic alkaline-earths, as well (a bosonic alkaline-earth Mott insulator has already been achieved [24]). Furthermore, the requirement to reach $k_BT$ smaller than $J^2/U$ or $V_{ex}^2/J_g$ can often be relaxed. First, the double-well experiments, such as the ones discussed in the Methods in the contexts of the Kugel-Khomskii and the double-well experiments, such as the ones discussed in the Methods in the contexts of the Kugel-Khomskii and the Kondo lattice model, are performed out of thermal equilibrium, and can, thus, access energy scales far below the temperature of the original cloud [39]. Second, for SU(N) antiferromagnets, the energy range between $J^2/U$ and $N/J^2/U$ may also exhibit intriguing physics: in this regime, SU(N) singlets, which require $N J^2/U$ energy to break, stay intact but can diffuse around. Finally, in the $V_{ex} < 0$ Kondo lattice model, exotic heavy Fermi liquid behavior is expected when $J_g \lesssim |V_{ex}|$ and the temperature is below the Kondo temperature, i.e., $k_BT \lesssim J_g \exp(-c J_g/|V_{ex}|)$ with $c$ is a dimensionless constant of order one [25]. Thus, with $J_g$ chosen to be on the order of $|V_{ex}|$, $k_BT$ as high as $\sim |V_{ex}|$ may be sufficient.

Outlook

The proposed experiments should be regarded as bridges aiming to connect well-understood physics to the complex and poorly understood behavior of strongly correlated systems. It is important to emphasize that, except for the one dimensional case, the phase diagram of most of the models considered is only known at mean field level or numerically in reduced system sizes. Therefore, their experimental realization in clean and controllable ultracold atomic systems can provide major advances.

Our proposal motivates other new lines of research. Ultracold bosonic or fermionic diatomic molecules [45] may give rise to similar SU(N) models with large $N$ and with the possibility of long-range interactions. Ions with alkaline-earth-like structure, such as Al$^+$ could also be considered in this context. It would also be interesting to explore the possibility of realizing topological phases with SU(N) models for applications in topological quantum computation [34]. Beyond quantum magnetism, the fact that the formation of SU(N) singlets requires $N$ partners might give rise to novel exotic types of superfluidity and novel types of BCS-BEC crossover [37]. Practical applications of our Hubbard model, such as the calculation of the collisional frequency shift in atomic clocks [46], can also be foreseen.

Note added in proof. After the submission of this paper, a theoretical study of the SU(6)-symmetric $^{173}\text{Yb}$ system was reported [50].

Methods

Experimental tools available for alkaline-earth atoms

Many experimental tools, such as tuning the interaction strength by adjusting laser intensities [39], are common to both alkali and alkaline-earth atoms. There are, however, some experimental tools specific to alkaline earths; we review them in this Section.

First, a combination of optical pumping [2] and direct coherent manipulation of the $|g\rangle - |e\rangle$ transition in the presence of a magnetic field [1, 2] can be used [8] to prepare any desired single-atom state within the $2(2 I + 1)$-dimensional manifold with basis $|\alpha m\rangle$, where $\alpha = g$ or $e$ and $m = -I, \ldots, I$. This coherent manipulation can also be used to exchange quantum information between nuclear spin states and electronic states. Second, by using far-detuned probe light or a large magnetic field to decouple the electronic angular momentum $J$ and the nuclear spin $I$, the electronic $|g\rangle - |e\rangle$ degree of freedom can be measured by collecting fluorescence without destroying the nuclear spin state [3]. Fluorescence measurement of the nuclear spins can be achieved by mapping nuclear spin states onto electronic states [7, 8]: for example, for a spin-1/2 nucleus, a $\pi$ pulse between $|g, m = 1/2\rangle$ and $|e, m = -1/2\rangle$ allows one to accomplish a swap gate between the nuclear $\{1/2, -1/2\}$ qubit and the electronic $(e, g)$ qubit. Single-site spatial resolution during the coherent manipulation and fluorescence measurement can be achieved using magnetic field gradients [7] or dark-state-based techniques [8, 57] that rely on an auxiliary laser field whose intensity vanishes at certain...
locations. Third, an appropriate choice of laser frequencies allows one to obtain independent lattices for states $g$ and $e$ [7]. Finally, optical Feshbach resonances [48] may be used to control scattering lengths site-specifically and nearly instantaneously.

**Enhanced Symmetries**

While in the general case, our Hubbard model [Eq. (2)] satisfies $U(1) \times SU(N)$ symmetry, for particular choices of parameters, higher symmetry is possible. In particular, if $J_g = J_e$ and the interaction energies for all states within the pseudo-spin triplet are equal ($U_{gg} = U_{ee} = U_{eg}$), the full $SU(2)$ symmetry (not just $U(1)$) in the pseudo-spin space is satisfied. Alternatively, if $V_{ex} = 0$, then both $S_n^m(i,e)$ and $S_n^m(i,g)$ generate $SU(N)$ symmetries resulting in the overall $U(1) \times SU(N_g) \times SU(N_e)$ symmetry. Finally, if both conditions are satisfied, i.e. all four $U_X$ are equal and $J_g = J_e$, then $H$ satisfies the full $SU(2N)$ symmetry ($2N$ can be as high as 20) generated by

$$S_{j}^{m_{j}} = \sum_{j} S_{j}^{m_{j}}(j) = \sum_{j} c^{\dagger}_{j} \beta_{j} e^{i m_{j} \alpha_{j}},$$

where $\beta_{j} = \gamma_{j} + \gamma_{j'}$.

In the case when $|e\rangle$ and $|g\rangle$ correspond to two ground states of two different atoms (with nuclear spin $I_e$ and $I_g$, respectively), we will have $a_{eg}^{+} = a_{eg}^{-}$ (i.e $V_{ex} = 0$), which is equivalent to imposing $U(1) \times SU(N_g = 2I_g + 1) \times SU(N_e = 2I_e + 1)$ symmetry, where $SU(2I_\alpha + 1)$ is generated by $S_n^m(i,\alpha)$. While for $J_g \neq I_e$, the $m$ index in $c_{i\alpha m}$ will run over a different set of values depending on $\alpha$, the Hubbard Hamiltonian will still have the form of Eq. (2) (except with $V_{ex} = 0$). If one further assumes that $J_g = J_e$ and $U_{gg} = U_{ee} = U_{eg}$, the interaction satisfies the full $SU(N_g + N_e)$ symmetry. It is worth noting that for the case of two different ground state atoms, this higher symmetry is easier to achieve than for the case of two internal states of the same atom, since $a_{eg}^{+} = a_{eg}^{-}$ automatically. Thus, in particular, it might be possible to obtain $SU(18)$ with $^{87}$Sr ($I = 9/2$) and $^{43}$Ca ($I = 7/2$) simply by adjusting the intensities of the two lattices (to set $J_g = J_e$ and $U_{gg} = U_{ee}$) and then shifting the two lattices relative to each other (to set $U_{eg} = U_{gg}$).

Enhanced symmetries of the Hubbard model [Eq. (2)] are inherited by the spin Hamiltonian [Eq. (5)]. In particular, imposing $SU(2) \times SU(N)$ instead of $U(1) \times SU(N)$ forces $\kappa_{ge}^{ij} = \kappa_{eg}^{ij}, \kappa_{ge}^{ij} = \kappa_{eg}^{ij}, \kappa_{eg}^{ij} = \kappa_{ge}^{ij}, \kappa_{eg}^{ij} + \kappa_{ge}^{ij} = \kappa_{eg}^{ij}, \lambda_{ge}^{ij} = \lambda_{eg}^{ij}, \lambda_{ge}^{ij} = \lambda_{eg}^{ij}, \lambda_{eg}^{ij} = \lambda_{ge}^{ij} + \lambda_{ge}^{ij} = \lambda_{eg}^{ij}. \lambda_{ge}^{ij} = \lambda_{eg}^{ij} = 0$. Finally, imposing the full $SU(2N)$ forces the satisfaction of both sets of conditions, yielding

$$H = \sum_{\langle i,j \rangle} \left[ \kappa_{ij} n_i n_j + \lambda_{ij} S_{\alpha \beta m}(i) S_{\beta \alpha m}(j) \right],$$

which is, of course, equivalent to restricting Eq. (5) to $g$-atoms only and extending labels $m$ and $n$ to run over $2N$ states instead of $N$.

**Double-well Kugel-Khomskii and RKKY experiments**

In the main text and in the following Methods Section, we discuss the open questions and previously unexplored regimes associated with the SU(2) Hubbard-Model and Kondo lattice models (KLM) that can be studied with ultracold alkaline-earth atoms. As a stepping stone toward these many-body experiments, we propose in this Section two proof-of-principle experiments in an array of isolated double wells with $N = 2$ (with the spin basis $\{ \uparrow, \downarrow \}$): one to probe the spin-orbital interactions of the Kugel-Khomskii model and one to probe the RKKY interactions associated with KLM.

We first propose an experiment along the lines of Ref. [39] to prove the spin-orbital interactions giving rise to the $T = 0$ diagram in Fig. 3. In the Supplementary Information, we describe how to prepare an array of independent double wells in the state $|e\rangle |R\rangle \langle L| |e\rangle |R\rangle$, which is a superposition of the four eigenstates featured in Fig. 3. The energies of these four eigenstates [Eqs. (54)-(77)] can be extracted from the Fourier analysis of the population imbalance as a function of time: $\Delta N(t) = n_{eR} + n_{gL} - n_{gR} - n_{eL} = - \cos \left( \frac{4t J_{ex}}{\hbar U_{eg}} \right) - \cos \left( \frac{4t J_{ex}}{\hbar U_{eg}} \right)$. $\Delta N$ can be measured by combining the dumping technique, band mapping, and Stern-Gerlach labeling of Ref. [39] with the use of two probe laser frequencies to distinguish between $|g\rangle$ and $|e\rangle$.

We now turn to the double-well experiment aimed at probing RKKY interactions. After preparing the state $\frac{1}{\sqrt{2}} (|g\rangle \uparrow \downarrow + |g\rangle \downarrow \uparrow |e\rangle \downarrow \uparrow |e\rangle \uparrow \downarrow)$, the Neel order parameter for the $e$ atoms, $N_{ee} = \frac{1}{4} n_{e\downarrow} - n_{e\uparrow} - n_{e\uparrow} - n_{e\downarrow}$. In the limit $V_{ex} \ll J_g$, $N_{ee}(t) = - \frac{3}{4} \cos \left( \frac{V_{ex} t}{\hbar} \right) - \frac{1}{2} \cos \left( \frac{V_{ex} t}{\hbar} - \frac{3V_{ex}^2}{8J_g} \right)$ [in the Supplementary Information, we present the plot of $N_{ee}(t)$ for $V_{ex} = -J_g/10$]. It exhibits fast oscillations with frequency $\sim V_{ex}$, modulated by an envelope of frequency $\sim V_{ex}^2/J_g$ induced by RKKY interactions. In order to probe RKKY interactions only, it is important to suppress super-exchange $\sim J_g^2/U_{ex}$ and thus to choose $J_e/U_{ee}$ small. To study the full spatial dependence of RKKY interactions, one must of course go beyond the double-well setup. We also note that recent experiments using alkali atoms populating the lowest two vibrational levels of a deep optical lattice have measured the local singlet-triplet splitting induced by $V_{ex}$ [49].

**Physics accessible with the alkaline-earth Kondo lattice model**

The alkaline-earth atom realization of the AF KLM can be accessed using a number of parameter regimes that are out of reach in solid state materials. One example is the one dimensional (1D) limit, since, to our knowledge, real solid state materials exhibiting KLM physics are restricted to 2D or...
3D. Another example is the regime of large Kondo exchange ($|V_{ex}| \gg J_g$), which is interesting even for $N = 2$. In this limit the system is well described by the $U \rightarrow \infty$ Hubbard model [34] by identifying the Kondo singlets with empty sites (holes) and the unpaired localized spins with hard core electrons. From this mapping, possible ferromagnetic ordering is expected at small hole concentration (small $n_g$), however the stability of this phase for increasing hole concentration and finite $|V_{ex}|$ values remains unknown. For general $N$, in the extreme limit $J_g = 0$, the ground state is highly degenerate: for any distribution of the $g$ atom density $n_{gg} < N$, there is a ground state (with further spin degeneracy), where on each site the spins combine antisymmetrically to minimize the exchange interaction. Lifting of such extensive degeneracies often leads to novel ground states; this will be addressed in future studies using degenerate perturbation theory in $J_g/V_{ex}$.

For $N > 2$, AF SU(N) spin models have a different kind of extensive degeneracy, which was argued to destroy antiferromagnetism and to lead to non-magnetic spin liquid and VBS-like ground states [34]. Similar expectations are likely to apply to the KLM at small $|V_{ex}|/J_g$, where the $N = 2$ antiferromagnetism may give way to situations where the localized spins form a non-magnetic state that is effectively decoupled from the mobile fermions [23].

Even though we have set $U_{gg}$ to zero in Eq. (5), it can be tuned, for example, by adjusting the $g$-lattice depth and can give rise to interesting physics. For example, the $n_g = 1$ case, which is known to be for $N = 2$ either an antiferromagnetic insulator or a Kondo insulator depending on the ratio $|V_{ex}|/J_g$ [19], will become for large enough $U_{gg}$ and $N > 2$ a Mott insulator, because the two atoms on each site cannot combine to form an SU(N) singlet. If $n_g$ is reduced from unity, the doping of this Mott insulator can be studied, and it will be interesting to understand how this physics, usually associated with cuprate superconductors, is related to the other ground states of the KLM, usually associated with heavy fermion compounds.

Experimental Accessibility

Immediate experimental accessibility makes our proposal particularly appealing. Having shown in the main text that the temperature requirements of our proposal are within reach of current experimental systems, here we show that the nuclear-spin dependence of interaction energies is sufficiently weak to keep the SU(N) physics intact.

In the Supplementary Information, nuclear-spin-dependent variation in the interaction energies is estimated to be $\Delta U_{gg}/U_{gg} \sim 10^{-9}$ and $\Delta U_{ee}/U_{ee} \sim \Delta U_{eg}/U_{eg} \sim 10^{-3}$. Since the scale of SU(N) breaking is at most $\Delta U$, a very conservative condition for the physics to be unaffected by SU(N) breaking is that all important energy scales are greater than $\Delta U$. In particular, in the spin models with more than one atom per site, the condition is $\Delta U \ll J^2/U$, which can be satisfied simultaneously with $J \ll U$ even for $\Delta U/U \sim 10^{-3}$. With one atom per site, the SU(N) breaking scale is not $\Delta U$ but rather $(J/U)^2 \Delta U$, which relaxes the condition to the immediately satisfied $\Delta U/U \ll 1$. Similarly, in the Kondo lattice model, the conditions $\Delta V_{ex} \ll J, |V_{ex}|$ can be satisfied for $\Delta V_{ex}/|V_{ex}| \sim 10^{-3}$.

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Author contributions

All authors contributed extensively to the work presented in this paper.

Additional information

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SUPPLEMENTARY ONLINE MATERIALS

Known Scattering Lengths

Very few scattering lengths $a_X (X = gg, ee, eg^+, eg^-)$ between $g (1S_0)$ and $e (3P_0)$ states of alkaline-earth-like atoms are known at the moment. $a_{gg}$ is known for all isotopic combinations of Yb [51] and Sr [52]. Estimates of $a_{ee}$ for $^{88}$Sr [53] and of $a_{eg}$ for $^{87}$Sr [54] also exist. Finally, there is a proposal describing how to measure $a_{eg}^+$ via clock shifts [55].

Nuclear-Spin Independence of the Scattering Lengths

Independence of scattering lengths from the nuclear spin is a key assumption of the paper. This feature allows us to obtain SU(N)-symmetric models with $N$ as large as 10 and distinguishes alkaline-earth atoms from alkali atoms, which can exhibit at most an SO(5) symmetry [56, 57, 58, 59], a symmetry that is weaker than SU(4). The assumption of nuclear-spin independence of scattering lengths is consistent with recent experiments, where - within experimental precision - the clock independence of scattering lengths is consistent with recent estimates [60] of $\alpha_{eg}$ for $^{138}$Ba as $\sim 10^{-7}$ for $a_{eg}$ and $\sim 10^{-8}$ for $a_{ee}$.

Turning to the actual numbers, $\Delta t$ can be estimated from the depth ($\sim 10^3 \text{cm}^{-1} \hbar c$) and the range ($\sim 10 \text{ Bohr radii}$) of the appropriate interatomic potential (see e.g. [63, 64]) to be $\Delta t \approx 1 \text{ ps}$. For $g$-$g$ collisions, $\delta V / \hbar$ can be estimated by the second-order formula $E_{\text{opt}} \sim 200 \text{ Hz}$, where $E_{\text{opt}} / \hbar \sim 300 \text{ MHz}$ is the approximate value for the hyperfine splittings in $^3P_1$ in $^{87}$Sr and $E_{\text{opt}} / \hbar \sim 400 \text{ THz}$ is the optical energy difference between $^1S_0$ and $^3P_1$ in $^{87}$Sr. This yields the following estimate for the dependence of $\alpha_{gg}$ on the nuclear spin: $\delta a_{gg} / a_{gg} \sim \delta \Phi / \hbar \sim 10^{-9}$. For $e$-$e$ and $e$-$g$ collisions, an analogous second-order formula would use the fine structure splitting between $^3P_1$ and $^3P_0$ in $^{87}$Sr ($E_{\text{opt}} / \hbar \sim 6 \text{ THz}$) instead of $E_{\text{opt}}$ to yield $\delta a_{eg} / a_{eg} \sim 10^{-5}$. However, the latter estimate ($\delta a_{eg} / a_{eg} \sim 10^{-5}$) is too optimistic since molecular states that are split by $E_1$ at large interatomic separations may come orders of magnitude closer at short range [60]. Therefore, a more realistic conservative estimate would use the first-order formula $\delta V \sim E_{\text{opt}}$ to yield $\delta a_{ee} / a_{ee} \sim \delta a_{eg} / a_{eg} \sim \delta \Phi / \hbar \sim 10^{-3}$. It is important to note, however, that these are all only very rough estimates. For example, hyperfine coupling in a molecule will differ from the hyperfine coupling in separated atoms. In fact, since it is very difficult to predict $\delta a / a$ accurately, these values would need to be measured. To conclude this Section, we would like to emphasize that, as mentioned in the main text, if the small nuclear-spin dependence of $a_{ee}$ and $a_{eg}$ is not negligible for some applications, one can use two different ground state atomic species instead of a ground and an excited state of one species.

Likelihood of Lossy $e$-$e$ Collisions and Possible Solutions

Collisions of two $e$ atoms are likely to be accompanied by large loss [53]. This can occur if the molecular $\Omega e^2$ potential that correlates with the $e$-$e$ states undergoes an avoided crossing with a potential curve that correlates with a lower energy pair of separated atoms (see, for example, Ref. [64]). Similar crossings that result in inelastic energy transfer collisions were examined for $^3P_1 + ^1S_0$ collisions of alkaline earth atoms in Ref. [67]. The likelihood of a relatively high probability of an inelastic event during such a crossing with species such as Sr or Yb means that the imaginary part $b_{ee}$ of the scattering length is expected to be large. However, just like $a_{ee}$, $b_{ee}$ can not be calculated accurately from the potentials but would need to be measured.

The possible effects of $b_{ee}$ on the four examples we discuss...
[Eqs. (68) and Eq. (S1)] are as follows. $H_{(p,0)}$ [Eq. (7)] is, of course, not affected because it involves only $g$ atoms. In $H_{(1,1)}$ [Eq. (S1)] and $H_{KLM}$ [Eq. (8)], the $e$ lattice is assumed to be so deep that $J_e$ is negligible compared to $U_{ee} + V_{ex}$ and $U_{ee}$, respectively, or to the experimental timescale, thus, fully suppressing tunneling of $e$ atoms and occupation of one site by more than one $e$ atom. The presence of an imaginary part $b_{ee}$ of the $e$-$e$ scattering length will give an effective nonzero width to the state with more than one $e$ atom per site and can, therefore, only further suppress this tunneling by a Zeno-like effect [68, 69, 70].

Therefore, $H_{(1,0)}$ [Eq. (6)] is the only example that can be affected by large $b_{ee}$. In order for $H_{(1,0)}$ to contain a non-negligible term proportional to $J_e^2/U_{ee}$, the ratio $|b_{ee}/a_{ee}|$ would need to be very small [71]. Several approaches to avoid the losses associated with $b_{ee}$ in $H_{(1,0)}$ are possible. First, the large variety of stable atoms with two valence electrons (which includes not only alkaline-earths, but also Zn, Cd, Hg, and Yb) may have coincidentally an isotope with $a_{ee}$ small [51, 72, 73, 74, 75] to reduce $|b_{ee}/a_{ee}|$ and, thus, suppress $b_{ee}$ and, thus, suppress $H_{(1,0)}$. Several approaches to avoid the losses associated with $b_{ee}$ in $H_{(1,0)}$ are possible. First, the large variety of stable atoms with two valence electrons (which includes not only alkaline-earths, but also Zn, Cd, Hg, and Yb) may have coincidentally an isotope with small $|b_{ee}/a_{ee}|$, which is more likely for lighter atoms [67].

Second, while obtaining a good optical Feshbach resonance [51, 72, 73, 74, 75] to reduce $|b_{ee}/a_{ee}|$ might not be possible, it should be possible to use optical Feshbach resonances to enhance $b_{ee}$ and, thus, suppress $H_{(1,0)}$. It can be obtained when there is one $g$ and one $e$ atom per site in the electronic singlet $|ge⟩ - |eg⟩$ configuration. Setting $J_e = 0$ to avoid $e$-$e$ collisions, $H_{(p,q)}$ reduces to

$$H_{(1,1)} = \frac{J_e^2}{2(U_{gg} + V_{ex})} \sum_{i,j} S_{ij}^2.$$  

The case of $N = 2$ is the spin-1 antiferromagnetic Heisenberg model. This model has a 1D ground state with hidden topological structure [78]. Recently, applications of related models in one-way quantum computation have been proposed [79, 80]. Models with more complicated two-column representations may have exotic chiral spin liquid ground states that support non-Abelian anyons and that might thus be used for topological quantum computation [81].

**Brief Review of Young Diagrams**

Irreducible representations of SU(2) are classified according to the total half-integer angular momentum $J$ and have dimension $2J + 1$. On the other hand, a (semistandard) Young diagram, instead of a single value $J$, is used to describe an irreducible representation of SU(N) for a general $N$ [76, 77]. As shown in the example in Fig. S1, a Young diagram has all its rows left-aligned, has the length of rows weakly decreasing from top to bottom, and has at most $N$ rows. The dimension of the representation corresponding to a given diagram is the number of ways to fill the diagram with integers from 1 to $N$ such that the numbers weakly increase across each row and strictly increase down each column. For our purposes, the number of boxes in the diagram is the number of atoms on the site, and the diagram describes the (nuclear) spin symmetry of the particular chosen single-site energy manifold. In particular, columns represent antisymmetrized indices, while rows are related to (but do not directly represent) symmetrized indices. It is the relation between antisymmetrized indices and the columns that limits the number of rows to $N$. On the other hand, since the full wavefunction (spin and orbital) on each site must satisfy complete fermionic antisymmetry, the relation between rows and symmetrized indices and the fact that we have only two orbital states ($g$ and $e$) force all our diagrams to have at most two columns.

**The (p, q) = (1, 1) spin Hamiltonian and the spin-1 Heisenberg antiferromagnet**

In the main text, we discussed two special cases of the spin Hamiltonian $H_{(p,q)}$, both of which had a single-column SU(N) representation on each site (i.e. $q = 0$). In this Section, we discuss the simplest SU(N) representation with two columns, $(p,q) = (1,1)$ [see Fig. S2]. It can be obtained when there is one $g$ and one $e$ atom per site in the electronic singlet $|ge⟩ - |eg⟩$ configuration. Setting $J_e = 0$ to avoid $e$-$e$ collisions, $H_{(p,q)}$ reduces to

$$H_{(1,1)} = \frac{J_e^2}{2(U_{gg} + V_{ex})} \sum_{i,j} S_{ij}^2.$$  

The case of $N = 2$ is the spin-1 antiferromagnetic Heisenberg model. This model has a 1D ground state with hidden topological structure [78]. Recently, applications of related models in one-way quantum computation have been proposed [79, 80]. Models with more complicated two-column representations may have exotic chiral spin liquid ground states that support non-Abelian anyons and that might thus be used for topological quantum computation [81].

**The Kugel-Khomskii model and the double-well phase diagram**

In the main text, we omitted the values of the parameters in $H_{(p,q)}$ that characterize the Kugel-Khomskii model $H_{(1,0)}$ [Eq. (6)]. In this Section, we present these parameters. We also present a detailed discussion of the double-well case phase diagram.
The parameters in $H_{(g,q)}$ that characterize the Kugel-Khomskii model $H_{(1,0)}$ [Eq. (6)] are \( \lambda_{ij} = -\kappa_{ij} = \frac{2J_{ij}^2}{U_{ij}} \equiv -\kappa_{ij}, \lambda_{ge} = \frac{2J_{ge}^2}{U_{ge}} \equiv \kappa_{ge}, \lambda_{ge} = \frac{J_{ge}^2 + J_{yg}^2}{2U_{ge}} \equiv \lambda_{ge} \) separations.

The nontrivial orbital-orbital, spin-spin, and spin-orbital interactions in $H_{(1,0)}$ [Eq. (6)] result in competing orders, with the actual ground-state order dependent on the parameters of the Hamiltonian $H_{(1,0)}$. To get a sense of the possible orders, we consider the case $N = 2$ (with the spin states denoted by $\uparrow$ and $\downarrow$) and discuss the double-well problem, with the wells denoted by $L$ (left) and $R$ (right). Due to the large optical energy separating $e$ and $g$, which we have ignored after Eq. (1), the three manifolds of constant $T^z = T_L^z + T_R^z$ ($T^z = -1, 0, 1$) should each be considered separately.

The four states in the $T^z = 1$ manifold, the subspace of two $e$ atoms, are $|ee\rangle\langle s|$ and $|ee\rangle\langle t|$. Here $|ee\rangle = |ee\rangle_{LR}$ is the orbital (or pseudo-spin) state, while $|t\rangle = |\uparrow\uparrow\rangle_{LR} - |\downarrow\downarrow\rangle_{LR}$ and $|s\rangle = \frac{1}{\sqrt{2}}(|\uparrow\downarrow\rangle_{LR} + |\downarrow\uparrow\rangle_{LR})$ are the triplet and singlet spin states. Since $U_{ee} = \infty$, all four of these states have zero energy and the ground-state phase diagram is trivial.

The four states in the $T^z = -1$ manifold (two $g$ atoms) are split by $H_{(1,0)}$ into two energy manifolds:

\[
|gg\rangle\langle t|, \quad E = 0,
\]

\[
|gg\rangle\langle s|, \quad E = \frac{4J_{gg}^2}{U_{gg}}.
\]

Only $|gg\rangle\langle s|$ can take advantage of the virtual tunneling since two $g$ atoms in the triplet spin states cannot sit on the same site. Which of the two manifolds is the ground manifold depends on the sign of $U_{gg}$, as shown in the ground-state phase diagram in Fig. [S]. It is important to emphasize that for $U_{gg} < 0$, the subspace of one $g$ atom per site may be subject to extra loss down to the lower energy states that have both $g$ atoms in the same well. It is also worth noting that the diagram is only valid for $J_g \ll |U_{gg}|$.

Finally, the eight states in the $T^z = 0$ manifold (one $g$ atom and one $e$ atom) are split by $H_{(1,0)}$ into four energy manifolds:

\[
|\Sigma\rangle\langle t|, \quad E = -\frac{(J_g + J_e)^2}{U_{eg}},
\]

\[
|\tau\rangle\langle s|, \quad E = -\frac{(J_g + J_e)^2}{U_{eg}},
\]

\[
|\tau\rangle\langle t|, \quad E = -\frac{(J_g - J_e)^2}{U_{eg}},
\]

\[
|\Sigma\rangle\langle s|, \quad E = -\frac{(J_g - J_e)^2}{U_{eg}},
\]

where $|\Sigma\rangle = \frac{1}{\sqrt{2}}(|ee\rangle_{LR} - |ge\rangle_{LR})$ and $|\tau\rangle = \frac{1}{\sqrt{2}}(|ee\rangle_{LR} + |ge\rangle_{LR})$ are anti-symmetric and symmetric orbital states, respectively. The denominators $U_{eg}^-$ and $U_{eg}^+$ in the energies of the $|t\rangle$ and $|s\rangle$ states, respectively, reflect the fact that tunneling preserves the nuclear spin. At the same time, the $\pm$ signs in the numerators can be understood by considering the case $J_g = J_e$, when all states with overall symmetry under particle exchange must have zero energy since for these states tunneling is forbidden due to the Pauli exclusion principle. The corresponding ground-state phase diagram as a function of the signs and relative magnitude of $U_{eg}^+$ and $U_{eg}^-$ is shown in Fig. [S]. As in the case of the $T^z = 1$ phase diagram, negative interaction energies may lead to increased losses.

**Effects of Three-Body Recombination**

Three-body recombination \cite{74, 82, 83, 84, 85} is a process during which three atoms come together to form a diatomic bound state and a single atom, and both final products have enough kinetic energy to leave the trap. While in certain cases, three-body recombination can be an asset \cite{70}, usually it results in the loss of atoms and, thus, limits the duration of the experiment. For our purposes, we can describe three-body recombination by a decay rate $\gamma_3$ \cite{70} resulting in a loss of three particles from one site. This rate will likely depend on what atomic states are involved and, to the best of our knowledge, has not yet been measured or calculated for fermionic alkaline-earth atoms.

Out of the four examples [Eqs. (6),8 and Eq. (8)] that we discuss, only $H_{(1,1)}$ [Eq. (S1)] and $H_{(p,0)}$ [Eq. (7)] may be affected by three-body recombination ($H_{KLM}$ [Eq. (8)] assumes negligible $g$-$g$ interactions, such as in a very shallow $g$ lattice or with a low density of $g$ atoms). In the case of $H_{(1,1)}$, two $g$ atoms and one $e$ atom occupy the same site virtually in the intermediate state that gives rise to the second order spin Hamiltonian with interaction strength $\propto J_{gg}/(U_{gg} + V_{ex})$. Thinking of $\gamma_3$ as an effective linewidth for the intermediate state, $H_{(1,1)}$ will be valid and losses small provided that $\gamma_3$ is smaller than the effective "detuning" $U_{gg} + V_{ex}$. Since scattering lengths for alkaline-earth atoms \cite{51, 52, 54} are comparable to those for alkalai atoms, $U_{gg} + V_{ex}$ can be on the order of several kHz \cite{56}. At the same time, $1/\gamma_3$ for bosonic alkali atoms in deep traps can be on the order of $1 \times 10^4$. If $\gamma_3$ were the same in our case, $\gamma_3 \ll U_{gg} + V_{ex}$ would be satisfied. Ways of controlling the interactions via optical Feshbach resonances \cite{51, 52, 53, 54, 55} may also be envisioned.

In the case of $H_{(p,0)}$ [Eq. (7)], $(n_A, n_B) = (1,1)$ does not suffer from three-body recombination. $(n_A, n_B) = (1,2)$ and $(2,2)$ may have three atoms per site virtually. As in the discussion of $H_{(1,1)}$, provided $\gamma_3$ associated with three $g$ atoms per site is smaller than $U_{gg}$, these configurations should be accessible. For the case $(n_A, n_B) = (1,2)$, $\gamma_3 \gg U_{gg}$ is also acceptable, since it will effectively prohibit the tunneling of the atoms to the state with 3 atoms on a site \cite{74}, but the interaction can still take place through the intermediate state, in which an atom from a $B$ site tunnels to an $A$ site and back. One can also envision ways to use optical Feshbach resonances.
resonance techniques \cite{51, 72, 73} to induce large $\gamma_3$. To be able to resolve the superexchange coupling $\sim J_g^2/U_{gg}$ in cases where \( n_A \) or \( n_B \) is equal to 3, one must have $\gamma_3 < J_g^2/U_{gg}$. Given that superexchange coupling can be as high as 1 kHz \cite{62}, this condition should also be achievable. Although \( n_A \) or \( n_B \) greater than 3 will result in even shorter lifetimes \cite{84}, there is a good chance that relatively large \( n_A \) and \( n_B \) can be achieved: at least, for bosonic alkali atoms in an \( n = 5 \) Mott insulator state, the lifetime can still be as long as 0.2 s \cite{86}.

The \((p, 0)\) spin Hamiltonian with \( n_A = n_B \neq N/2 \)

In the main text, we focused on one special case of the antiferromagnetic \((p, 0)\) spin Hamiltonian on a square lattice, that with \( n_A + n_B = N \) (where \( n_A \) and \( n_B \) denote the number of atoms per site on the two sublattices). In this Section, we describe another interesting and experimentally relevant case, \( n_A = n_B \neq N/2 \). Potential ground states include states built from valence plaquettes (Fig. S3) \cite{81, 87, 88, 89, 90, 91, 92, 93}, resonant plaquette states \cite{87}, and topological spin liquids \cite{81, 90}. Valence plaquette states and resonant plaquette states are the natural generalization of VBS states and resonant valence bond states (RVB) \cite{94}, respectively; for example, when \( n_A = n_B = 1, N \) lattice sites are needed to form a SU\((N)\) singlet. Fig. S3 depicts a square lattice valence plaquette solid for \( n_A = n_B = 1 \) and \( N = 4 \). Techniques for detecting some of these phases are discussed in Ref. \cite{81}. The experiment described in the main text for the case \( n_A + n_B = N \) can also be generalized to probe the \( n_A = n_B \neq N/2 \) phase diagram including exotic phases such as valence plaquette solids (Fig. S3), as well as competing magnetically ordered states. The main difference is that after preparing a band insulator of \( N \) \( g \) atoms per site, each site should be split not necessarily into two sites but into the number of sites that is appropriate for the case being considered (e.g. 4 for the case shown in Fig. S3).

Double-well Kugel-Khomskii and RKKY experiments

In the Methods, we have omitted the description of how to prepare the initial states for the proof-of-principle double-well Kugel-Khomskii and RKKY experiments. We present this description in this Section.

We first describe how to prepare an array of independent double wells in the state \(|e, \uparrow\rangle_L |g, \downarrow\rangle_R\), which we use for the proof-of-principle experiment to probe the spin-orbital interactions in the Kugel-Khomskii model \cite{95, 96, 97, 98, 99, 100, 101}. After loading a band insulator of \(|g, \downarrow\rangle\) atoms in a deep optical lattice, an additional lattice for both \( g \) (green) and \( e \) (yellow) atoms with twice the spacing of the first lattice is turned on in one direction to create an array of independent double wells \cite{62}. Then, as shown in Fig. S4, in the presence of an \( e\)-lattice bias, \( \sigma^+ \) polarized light on resonance with the \(|g, \downarrow\rangle_L \rightarrow |e, \uparrow\rangle_L\) transition can be used to prepare the state \(|e, \uparrow\rangle_L |g, \downarrow\rangle_R\). For examples of earlier orbital physics studies with ultracold atoms, where the orbitals are distinguished only by the different motional states of the atoms, we refer the reader to Refs. \cite{102, 103, 104, 105, 106, 107} and references therein.

We now describe how to prepare the initial state \( \frac{1}{\sqrt{2}} (|g, \downarrow\rangle_L + |g, \downarrow\rangle_R) |e, \uparrow\rangle_L |e, \uparrow\rangle_R \) (see Fig. S5a) for the double-well proof-of-principle RKKY experiment, whose expected Nee order parameter \( N_{ee}(t) \) for \( V_{ex} = -J_g/10 \) is shown in Fig. S5b. The first step to prepare the initial state \( \frac{1}{\sqrt{2}} (|g, \downarrow\rangle_L + |g, \downarrow\rangle_R) |e, \uparrow\rangle_L |e, \uparrow\rangle_R \) is to load a band insulator with three \(|g, \downarrow\rangle\) atoms per site on the long lattice and then slowly ramp up the short lattice with a bias so that it is energetically favorable to have two atoms in the left well and one in the right well. Next one can change the state of the right atom from \(|g, \downarrow\rangle_R\) to \(|e, \uparrow\rangle_R\) by applying a \( \pi \) pulse of \( \sigma^+ \) polarized light resonant with this single-atom transition. The left well will be unaffected because the spectrum is modified by the interactions (if interactions alone do not provide the desired selectivity, one could, for example, change the bias of the \( e\)-lattice). The next step is to change the state of the left well from two \(|g, \downarrow\rangle_L\) atoms populating the lowest two vibrational states to \(|e, \uparrow\rangle_L |g, \downarrow\rangle_L\), both populating the lowest vibrational state. This can be accomplished by using \( \pi \)-polarized traveling wave laser light to apply a \( \pi \) pulse resonant with the transition between these two many-body states \cite{106}. This results in \(|e, \uparrow\rangle_L |g, \downarrow\rangle_L |e, \uparrow\rangle_R\). One can then
FIG. S5: Proof-of-principle experiment to probe RKKY interactions in an array of isolated double wells. a, Schematic representation of the initial state $\frac{1}{2}\sqrt{2}(\lowercase{\text{g}}\rangle\langle \lowercase{\text{l}} | L + \lowercase{\text{g}}\rangle\langle \lowercase{\text{l}} | R)\langle e, \lowercase{\text{e}} | L | e, \uparrow\rangle_R$. b, In the limit $|V_{ex}| \ll J_g$, the Neel order parameter for the $e$ atoms $|N_{ex}(t)| = \frac{1}{2}[n_{\text{g}L} - n_{\text{e}L} - (n_{\text{e}R} - n_{\text{g}R})]$ is

$$N_{ex}(t) \approx -\frac{1}{3} \cos \left( \frac{V_{ex}t}{\hbar} \right) - \frac{2}{3} \cos \left( \frac{V_{ex}t}{2\hbar} - \frac{3V_{ex}^2t^2}{8J_g^2} \right),$$

which is shown in red for $V_{ex} = -J_g/10$. It exhibits fast oscillations with frequency $\sim V_{ex}$, modulated by an envelope of frequency $\sim V_{ex}^2/J_g$ induced by RKKY interactions $(-\frac{1}{3} - \frac{2}{3} \cos \left( \frac{3V_{ex}^2t^2}{8J_g^2} \right)$ shown in blue).

[1-50] References for the main text are listed at the end of the main text above.

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