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Engineering the dynamics of effective spin-chain models for strongly interacting atomic gasesA. G. Volosniev,¹ D. Petrosyan,^{2,3} M. Valiente,⁴ D. V. Fedorov,¹ A. S. Jensen,¹ and N. T. Zinner¹¹*Department of Physics and Astronomy, Aarhus University, DK-8000 Aarhus C, Denmark*²*Aarhus Institute of Advanced Studies, Aarhus University, DK-8000 Aarhus C, Denmark*³*Institute of Electronic Structure and Laser, FORTH, GR-71110 Heraklion, Crete, Greece*⁴*SUPA, Institute of Photonics and Quantum Sciences, Heriot-Watt University, Edinburgh EH14 4AS, United Kingdom*

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We consider a one-dimensional gas of cold atoms with strong contact interactions and construct an effective spin-chain Hamiltonian for a two-component system. The resulting Heisenberg spin model can be engineered by manipulating the shape of the external confining potential of the atomic gas. We find that bosonic atoms offer more flexibility for independently tuning the parameters of the spin Hamiltonian through interatomic (intraspecies) interaction, which is absent for fermions due to the Pauli exclusion principle. Our formalism can have important implications for control and manipulation of the dynamics of few- and many-body quantum systems; as an illustrative example relevant to quantum computation and communication, we consider state transfer in the simplest nontrivial system of four particles representing exchange-coupled qubits.

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I. INTRODUCTION

Interacting many-body quantum systems harbor many paradigmatic quantum phenomena, such as superconductivity and quantum magnetism, but are difficult to treat theoretically. For strong interparticle interactions, the usual perturbative and many numerical methods are inadequate, requiring more sophisticated approaches. In the important case of one spatial dimension, relevant techniques include bosonization and the Tomonaga-Luttinger liquid theory [1] and the numerically powerful density-matrix renormalization group methods [2,3].

Cold atoms confined in magnetic and optical traps represent a remarkably clean and versatile system to simulate and study many-body physics under well-controlled conditions [4–8]. Optical lattice potentials allow realization of the fundamental Hubbard model [9,10] in which quantum phase transition to the Mott insulator state with a single atom per lattice site has been demonstrated [11–13]. The Mott-Hubbard insulator for a two-component system can be mapped onto the Heisenberg spin Hamiltonian [14,15], facilitating studies of interacting spin models responsible for many key features of quantum magnetism [16]. One-dimensional (1D) systems of strongly interacting bosons [17–20] and fermions [21,22] have recently become experimentally accessible.

Experiments to simulate various lattice models with cold atoms typically involve a weak trapping potential superimposed onto the optical lattice [5]. The resulting potential deviates from an idealized homogeneous lattice, necessitating the use of the local-density approximation valid for a smooth trapping potential. Here we study an ensemble of cold alkali-metal atoms in an external trapping potential having an arbitrary shape (not necessary lattice) in the longitudinal direction but tightly confining the atoms in the transverse direction, realizing thereby an effective 1D system. A pair of internal atomic states from the ground-state hyperfine (Zeeman) manifold play the role of the spin-up and spin-down states. We show that such a 1D ensemble of strongly interacting atoms with *any* external confinement can, quite generally, be represented as a spin chain. The strong contact interatomic

interaction results in spatial localization of individual atoms within segments along the 1D trap, while the small but finite overlap between the wave functions of neighboring atoms leads to an effective spin-exchange interaction. We construct an effective spin- $\frac{1}{2}$ XXZ model for a two-component system and show that the parameters of the corresponding Hamiltonian sensitively depend on the shape of the confinement potential, quantum statistics of the constituent atoms (bosons or fermions), and the interatomic interaction (for bosons only). We note an early relevant publication [23] deriving an effective Heisenberg spin- $\frac{1}{2}$ Hamiltonian for the homogeneous, large- U Hubbard model at low filling, and the very recent mapping of a multicomponent cold atomic gas in a harmonic trap onto a spin-chain model [24].

Our results open several possibilities for engineering stationary and dynamic quantum states of few- and many-body systems. As a revealing example amenable to analytic treatment, we consider the problem of quantum-state transfer [25–27] in the simplest yet nontrivial case of four particles. We show that by an optimal choice of the trapping potential and intraspecies interactions between bosonic atoms, perfect transfer [28–30] of a state of quantum bit, or qubit, between the two ends of the spin chain can be attained. By contrast, fermions cannot accommodate perfect state transfer, unless they are subject to local (effective) magnetic fields.

The paper is organized as follows. In the next section, we demonstrate the equivalence of the eigenspectra of a two-component ensemble on N atoms in a 1D trap and a corresponding spin chain. In Sec. III we study the dependence of the parameters of the effective spin Hamiltonian on the shape of the external trapping potential for the atoms. Quantum dynamics and state transfer in engineered chains of four spins is illustrated in Sec. IV, followed by concluding remarks in Sec. V. In the Appendix we present a perturbative derivation of the energy eigenvalues of the system using the approach of Ref. [31], analytic expressions for the eigenspectrum of a four-spin system and dynamics of quantum-state transfer, and derivation of an effective Heisenberg spin model in a magnetic field.

II. EFFECTIVE SPIN-CHAIN MODEL FOR N ATOMS

Consider a 1D system of N_\uparrow particles of one kind (spin up) and N_\downarrow particles of another kind (spin down) confined by an external trapping potential $V(x)$ with a characteristic length scale L . The total Hamiltonian for $N = N_\uparrow + N_\downarrow$ particles is given by

$$H = \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^{N_\sigma} \left[h(x_{\sigma,i}) + \frac{g_{\sigma\sigma}\hbar^2}{mL} \sum_{i'>i}^{N_\sigma} \delta(x_{\sigma,i} - x_{\sigma,i'}) \right] + \frac{g_{\uparrow\downarrow}\hbar^2}{mL} \sum_{i=1}^{N_\uparrow} \sum_{i'=1}^{N_\downarrow} \delta(x_{\uparrow,i} - x_{\downarrow,i'}), \quad (1)$$

where

$$h(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{mL^2} V(x/L) \quad (2)$$

is the single-particle Hamiltonian, m is the mass assumed equal for all particles, and $x_{\uparrow(\downarrow),i}$ denotes the position of the i th spin-up (spin-down) particle. Throughout this paper, we use L and $\varepsilon \equiv \frac{\hbar^2}{mL^2}$ as units of length and energy, respectively. The zero-range interactions are parametrized by the dimensionless strengths $g_{\uparrow\downarrow} \equiv g > 0$ and $g_{\downarrow\downarrow} = g_{\uparrow\uparrow} \equiv \kappa g$ with $\kappa > 0$. Hamiltonian (1) applies to both bosons and fermions, but the total wave function should be symmetric for bosons and antisymmetric for fermions. As a consequence, identical (same-spin) fermions do not interact.

We assume strong interactions, $g \gg 1$, and inspect the N -particle wave functions $\Phi(\{x_{\uparrow,i}, x_{\downarrow,i'}\})$ for various configurations $\{x_{\uparrow,i}, x_{\downarrow,i'}\}$ of atomic positions. There are, in fact, $\binom{N}{N_\uparrow} = \frac{N!}{N_\uparrow! N_\downarrow!}$ distinguishable configurations with different ordering of atoms (spins), e.g., $x_{\uparrow,1} < x_{\uparrow,2} < x_{\downarrow,1} < \dots < x_{\uparrow,N_\uparrow} < \dots < x_{\downarrow,N_\downarrow}$. In the limit of $1/g \rightarrow 0$, the requirement of finite energy implies that Φ should vanish whenever the coordinates of any two particles coincide, $x_{\uparrow(\downarrow),i} = x_{\uparrow(\downarrow),i'}$. This requirement can only be satisfied if Φ is proportional to the Slater determinant wave function for N particles [31,32], which is a completely antisymmetric superposition of the products of different single-particle wave functions representing solutions of the single-particle Hamiltonian $h(x)$. In what follows, we assume that the potential V supports at least N bound single-particle levels, which are nondegenerate; the case of a (partially) degenerate spectrum can be treated similarly [31].

Consider the Slater determinant wave function Φ_0 composed of the N lowest-energy single-particle eigenfunctions of $h(x)$. For $1/g \rightarrow 0$, all $M(N_\uparrow, N_\downarrow) \equiv \binom{N_\uparrow + N_\downarrow}{N_\uparrow}$ configurations of atomic coordinates yield the same energy E_0 for $\Phi_0(\{x_{\uparrow,i}, x_{\downarrow,i'}\})$. We can expand the general N -particle eigenfunction as

$$\Psi = \sum_{k=1}^{M(N_\uparrow, N_\downarrow)} a_k \Pi_k \Phi_0(\{x_{\uparrow,i}, x_{\downarrow,i'}\}), \quad (3)$$

where $\{x_{\uparrow,i}, x_{\downarrow,i'}\} \equiv x_{\uparrow,1} < \dots < x_{\uparrow,N_\uparrow} < x_{\downarrow,1} < \dots < x_{\downarrow,N_\downarrow}$, and the sum is over all the permutations Π_k of coordinates. Note that for $1/g = 0$ any set of coefficients a_k defines a legitimate ground state, and we have in fact $M(N_\uparrow, N_\downarrow)$ mutually independent ground states of the same energy E_0 .

For small but finite $1/g$, the degeneracy of this ground-state manifold is lifted, which follows from the Hellmann-Feynman theorem [31,33]:

$$\frac{\partial E}{\partial g} = \kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^{N_\sigma} \sum_{i'>i}^{N_\sigma} \langle \Psi | \delta(x_{\sigma,i} - x_{\sigma,i'}) | \Psi \rangle + \sum_{i=1}^{N_\uparrow} \sum_{i'=1}^{N_\downarrow} \langle \Psi | \delta(x_{\uparrow,i} - x_{\downarrow,i'}) | \Psi \rangle. \quad (4)$$

Using the wave function of Eq. (3), we then obtain (see Appendix A) the corresponding energy, to linear order in $1/g$, as

$$E = E_0 - \frac{\sum_{j=1}^{N-1} \frac{\alpha_j}{g} (A_j + \frac{2}{\kappa} C_j + \frac{2}{\kappa} D_j)}{\sum_{k=1}^{M(N_\downarrow, N_\uparrow)} a_k^2}, \quad (5)$$

where

$$A_j = \sum_{k=1}^{M(N_\downarrow-1, N_\uparrow-1)} (a_{j|k} - b_{j|k})^2, \\ C_j = \sum_{k=1}^{M(N_\downarrow, N_\uparrow-2)} c_{j|k}^2, \quad D_j = \sum_{k=1}^{M(N_\downarrow-2, N_\uparrow)} d_{j|k}^2,$$

for bosons, while $C_j = D_j = 0$ for fermions. Here $a_{j|k}$ denotes the a_k coefficients in the expansion (3) multiplying terms $\Phi_0(\dots < x_{\uparrow,j} < x_{\downarrow,j+1} < \dots)$, with x_{\uparrow} at position j followed by x_{\downarrow} at position $j+1$, while $b_{j|k}$ are the coefficients of $\Phi_0(\dots < x_{\downarrow,j} < x_{\uparrow,j+1} < \dots)$, with x_{\uparrow} and x_{\downarrow} swapped. Similarly, for identical bosons, $c_{j|k}$ denote the expansion coefficients in Eq. (3) in front of $\Phi_0(\dots < x_{\uparrow,j} < x_{\uparrow,j+1} < \dots)$, while $d_{j|k}$ are the coefficients of $\Phi_0(\dots < x_{\downarrow,j} < x_{\downarrow,j+1} < \dots)$. Finally, the geometric factors α_j are solely determined by the confining potential through Φ_0 as

$$\alpha_j = \frac{\int \prod_{i=1}^{N_\uparrow} dx_{\uparrow,i} \prod_{i'=1}^{N_\downarrow} dx_{\downarrow,i'} \left| \frac{\partial \Phi_0}{\partial x_{\downarrow,j}} \right|^2 \delta(x_{\uparrow,j} - x_{\downarrow,j+1})}{\int \prod_{i=1}^{N_\uparrow} dx_{\uparrow,i} \prod_{i'=1}^{N_\downarrow} dx_{\downarrow,i'} |\Phi_0(\{x_{\uparrow,i}, x_{\downarrow,i'}\})|^2}, \quad (6)$$

where in Φ_0 in the numerator the spin-down atom $x_{\downarrow,j+1}$ is placed at position $j+1$ following j spin-up atoms $x_{\uparrow,1} \dots x_{\uparrow,j}$. Below we deal mostly with bosons, as they can also reproduce fermions in the limit of $\kappa \rightarrow \infty$.

We now demonstrate that Hamiltonian (1) for $N = N_\uparrow + N_\downarrow$ strongly interacting particles, $1/g \ll 1$, can be mapped onto the spin- $\frac{1}{2}$ XXZ Hamiltonian of the form

$$H_s = E_0 \mathbf{I} - \frac{1}{2} \sum_{j=1}^{N-1} \left[J_j (\boldsymbol{\sigma}^j \boldsymbol{\sigma}^{j+1} - \mathbf{I}) - \frac{2J_j}{\kappa} (\sigma_z^j \sigma_z^{j+1} + \mathbf{I}) \right], \quad (7)$$

where \mathbf{I} is the identity matrix, $\boldsymbol{\sigma}^j = (\sigma_x^j, \sigma_y^j, \sigma_z^j)$ are the Pauli matrices acting on the spin at site j , and J_j are position-dependent interaction coefficients. Note that H_s conserves the total spin projection, $\Sigma_z = N_\uparrow - N_\downarrow$.

Any eigenstate of (7) can be expanded in terms of the spin permutations Π_k as

$$|\Psi\rangle = \sum_{k=1}^{M(N_\uparrow, N_\downarrow)} a_k \Pi_k |\uparrow_1 \cdots \uparrow_{N_\uparrow} \downarrow_1 \cdots \downarrow_{N_\downarrow}\rangle. \quad (8)$$

Consider the energy expectation value $\langle\Psi|H_s|\Psi\rangle$. Using the swap operator $\mathbf{P}_{j,j+1} = \frac{1}{2}(\boldsymbol{\sigma}^j \boldsymbol{\sigma}^{j+1} + \mathbf{I})$, we find that the nonzero contributions to $\frac{1}{2}\langle\Psi|\boldsymbol{\sigma}^j \boldsymbol{\sigma}^{j+1} - \mathbf{I}|\Psi\rangle$ are

$$[a_{j|k}\langle\Phi_{j|k}| + b_{j|k}\langle\Phi_{j|k}|\mathbf{P}_{j,j+1}\rangle(\mathbf{P}_{j,j+1} - \mathbf{I})a_{j|k}\langle\Phi_{j|k}| + b_{j|k}\mathbf{P}_{j,j+1}|\Phi_{j|k}\rangle] = -a_{j|k}^2 - b_{j|k}^2 + 2a_{j|k}b_{j|k},$$

where $|\Phi_{j|k}\rangle \equiv |\cdots \uparrow \downarrow \cdots\rangle_{j,j+1}$. Assuming normalization $\langle\Psi|\Psi\rangle = 1$, we then obtain

$$\langle\Psi|H_s|\Psi\rangle = E_0 + \sum_{j=1}^{N-1} J_j \left(A_j + \frac{2}{\kappa} C_j + \frac{2}{\kappa} D_j \right), \quad (9)$$

with A_j , C_j , and D_j having the same meaning as above. Comparison of Eqs. (5) and (9) reveals that, to linear order in $1/g$, the eigenvalue problem for the Hamiltonians (1) and (7) is the same, with the corresponding spin-spin interaction coefficients given by $J_j = -\alpha_j/g$. Note that since the overlap integrals α_j are always positive, the coefficients J_j are negative, which is to be expected for a strongly repulsive interatomic interaction $g > 0$. (This is similar to the optical lattice setup [14], where the spin-spin interactions are mediated by virtual intermediate two-atom states having higher energy and therefore pushing the energies of single-atom states down.) For fermions or hard-core bosons, $\kappa \rightarrow \infty$, Eq. (7) becomes the XXZ Hamiltonian, while in the special case of bosons with $\kappa = 2$, it reduces to the XX model Hamiltonian. These results are summarized in Table I. In Ref. [24] Deuretzbacher *et al.* also arrive at a spin-model Hamiltonian for a harmonically trapped two-component atomic gas of fermions with $\kappa \rightarrow \infty$ and bosons with $\kappa = 1$.

For concreteness, we have contemplated so far only the ground-state energy manifold of Hamiltonian (1), yet precisely the same arguments apply to any n th-excited-state manifold, which can be represented by a corresponding XXZ Hamiltonian (7) disconnected from all the other energy manifolds, each located in the vicinity of energy E_n of the corresponding Slater determinant wave function Φ_n . This of course holds for small enough time scales when we can neglect energy relaxations, finite temperature, and other effects causing transitions between different energy manifolds E_n of the system.

TABLE I. Effective Heisenberg spin models for strongly interacting atoms in 1D traps.

Spin- $\frac{1}{2}$ model	Constituents	κ
XXZ	Bosons	$0 < \kappa < \infty$
XXX	Bosons or fermions	$\kappa \rightarrow \infty$
XX	Bosons	$\kappa = 2$

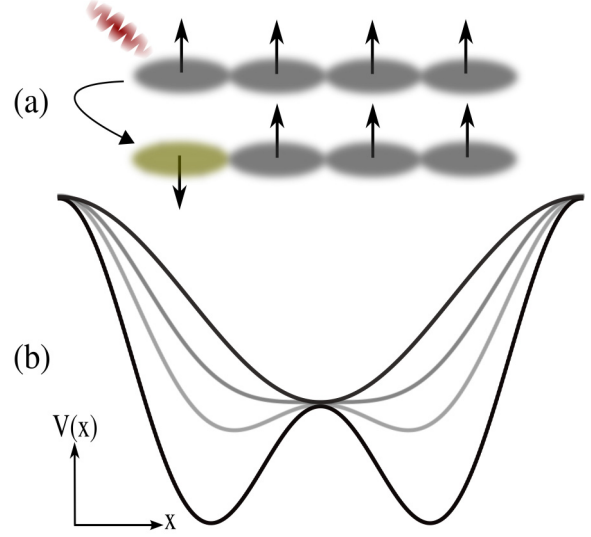


FIG. 1. (Color online) (a) A system of four atoms in a 1D trap is initialized by changing the internal state (flipping spin) of one of the atoms. (b) Trapping potential of Eq. (10) for $V_0 = 50\varepsilon$ and $u = (0, 1, 2, 4) \times u_p$ (top to bottom) with $u_p \simeq 12.5\varepsilon$.

III. CONTROLLING THE SPIN-CHAIN HAMILTONIAN

The above analysis attests to the possibility of tuning the interspin couplings J_j and anisotropy of the effective Hamiltonian H_s , Eq. (7), through the trapping potential $V(x)$ and interparticle interactions $g \gg 1$ and $\kappa > 0$. As an illustration, consider a relatively simple yet nontrivial system of four particles confined in a symmetric double-well trap of the form (see Fig. 1)

$$V(x) = -V_0 \sin^2 \left[\frac{1}{2}(x+1)\pi \right] - u \sin^2 [(x+1)\pi]. \quad (10)$$

Varying parameter $u \geq 0$, we may change the potential whose depth $V_0 = 50\varepsilon$ is chosen large enough to accommodate at least four well-localized single-particle levels. This allows us to restrict the problem to $x \in [-1, 1]$ with hard wall boundaries at $|x| = 1$ and obtain accurate wave functions Φ_0 .

We assume that three of the particles are prepared in the internal (spin) state $|\uparrow\rangle$ and the fourth is in state $|\downarrow\rangle$ [Fig. 1(a)]. The system is then nontrivial, since the interspin coupling coefficients $J_1 (=J_3)$ and J_2 can be tuned independently, which is not possible for less than four particles in a symmetric trap. In Fig. 2 we show the dependence of energy eigenvalues λ_n of H_s and the ratio J_2/J_1 on the parameter u of the potential of Eq. (10). Clearly, for $u \ll V_0$ the potential $V(x)$ is nearly harmonic, leading to larger overlap of the wave functions of the particles in the middle of the trap, which results in $J_2/J_1 \simeq 1.4$. By increasing u we decrease the overlap and thereby the coupling strength J_2 relative to $J_{1,3}$ [see Fig. 2(d)]. For very large $u \gg V_0$, the system splits into two noninteracting parts with vanishing coupling J_2 in the middle and doubly degenerate eigenvalues. This tendency can be seen in Figs. 2(a)–2(c), where we use three representative values of κ . The fermionic case of $\kappa \rightarrow \infty$ corresponds to the isotropic spin Hamiltonian (see Appendix B 1). In the bosonic case with $\kappa < 1$, the interaction with the impurity (spin-down) particle is stronger than the interaction between identical

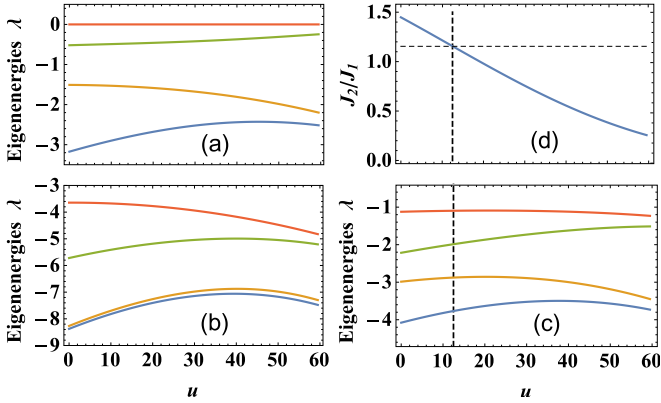


FIG. 2. (Color online) Energy eigenvalues λ_n of H_s (less the $E_0\mathbf{I}$ term) vs u of Eq. (10), for $N_\downarrow = 1$, $N_\uparrow = 3$ and (a) $\kappa \rightarrow \infty$ (fermions), (b) $\kappa = \frac{1}{2}$, and (c) $\kappa = 2$. The ratio J_2/J_1 of the coupling constants is shown in (d), with dashed lines marking $J_2/J_1 = \sqrt{4/3}$ and $u = u_p$, corresponding to the equidistant spectrum in (c). λ 's and u are in units of ε and $g = 100$.

(spin-up) particles. As a result, the pair of lowest-energy eigenstates, corresponding approximately to configurations $|\downarrow\uparrow\uparrow\uparrow\rangle \pm |\uparrow\uparrow\uparrow\downarrow\rangle$ with the impurity particle at the boundary, are almost completely decoupled from the other configurations and therefore are nearly degenerate (see Appendix B 2), which was also discussed in [34]. The case of $\kappa = 2$ corresponding to the XX model is of special interest in the following. As seen in Fig. 2(d), by choosing $u = u_p \simeq 12.5\varepsilon$ we obtain for the ratio of the coupling strengths $J_2/J_1 = \sqrt{4/3}$, leading to the equidistant eigenspectrum in Fig. 2(c).

IV. QUANTUM DYNAMICS IN ENGINEERED SPIN CHAINS

The possibility to realize various spin-chain Hamiltonians with cold-trapped atoms can have important implications for quantum simulations and computation [4,8]. A potentially useful application of quantum dynamics in engineered spin chains can be state transfer in small quantum networks [25–27]. Faithful transfer of quantum states is a prerequisite for achieving scalable quantum information processing in lattice-based schemes where qubit-qubit interactions are typically short range and implementing quantum logic gates between distant qubits requires interconnecting them via quantum channels represented by tunable spin chains [35].

In its standard form [25,26,35], the quantum-state transfer protocol involves preparing the spin chain in a dynamically passive state, e.g., $|\uparrow\uparrow\cdots\uparrow\uparrow\rangle$, and then initializing at time $t_{\text{in}} = 0$ the first spin with the qubit state $|\psi\rangle = \alpha|\uparrow\rangle + \beta|\downarrow\rangle$ to be transferred. Ideal transfer would imply that at a well-defined time t_{out} the last spin of the chain is in state $|\psi\rangle$ (up to a certain relative phase ϕ_0 between the amplitudes of $|\uparrow\rangle$ and $|\downarrow\rangle$). Since for the qubit state $|\uparrow\rangle$ the spin chain remains in the passive state, our aim is to maximize the probability of attaining state $|\uparrow\uparrow\cdots\uparrow\downarrow\rangle$ at time t_{out} given that at time $t = 0$ its state was $|\Psi(0)\rangle = |\downarrow\uparrow\cdots\uparrow\uparrow\rangle$. We thus define the fidelity of state transfer as

$$F(t) \equiv |\langle\Psi(t)|\uparrow\uparrow\cdots\uparrow\downarrow\rangle|^2. \quad (11)$$

The chain of four spins initialized as shown in Fig. 1(a) represents the smallest nontrivial system in which achieving perfect state transfer, $F(t_{\text{out}}) = 1$, requires a judicious choice of the parameters of Hamiltonian H_s . Indeed, in a two-state system, resonant coupling J_1 between $|\downarrow\uparrow\rangle$ and $|\uparrow\downarrow\rangle$ amounts to complete Rabi oscillations, while in a three-state system with degenerate initial $|\downarrow\uparrow\uparrow\rangle$ and final $|\uparrow\uparrow\downarrow\rangle$ states, and a not-too-large energy offset of the intermediate state $|\uparrow\downarrow\uparrow\rangle$, any J_1 and J_2 result in effective Rabi oscillations between the initial and final states [28,29]. The necessary and sufficient condition for perfect state transfer in a spin chain of any length N is a commensurate spectrum of H_s [30], namely, $e^{-i\lambda_n t_{\text{out}}} = (-1)^n e^{i\phi}$ with some ϕ , the equidistant spectrum, $\lambda_{n+1} - \lambda_n = \Delta\lambda \forall n$, being optimal [36] in terms of the fastest transfer time $t_{\text{out}} = \hbar\pi/\Delta\lambda$. In the case of the XX Hamiltonian, perfect and optimal state transfer is realized by choosing the coupling constants as $J_j = J_0\sqrt{(N-j)j}$ [28,29], resulting in $t_{\text{out}} = \hbar\pi/2J_0$. For our system of $N = 4$ spins, this corresponds to $J_2/J_1 = \sqrt{4/3}$ [see Figs. 2(c) and 2(d)] and transfer time $t_{\text{out}} = \hbar\pi/J_2$.

In Fig. 3 we show the time dependence of fidelities $F(t)$ of state transfer for the same values of κ as in Fig. 2. Due

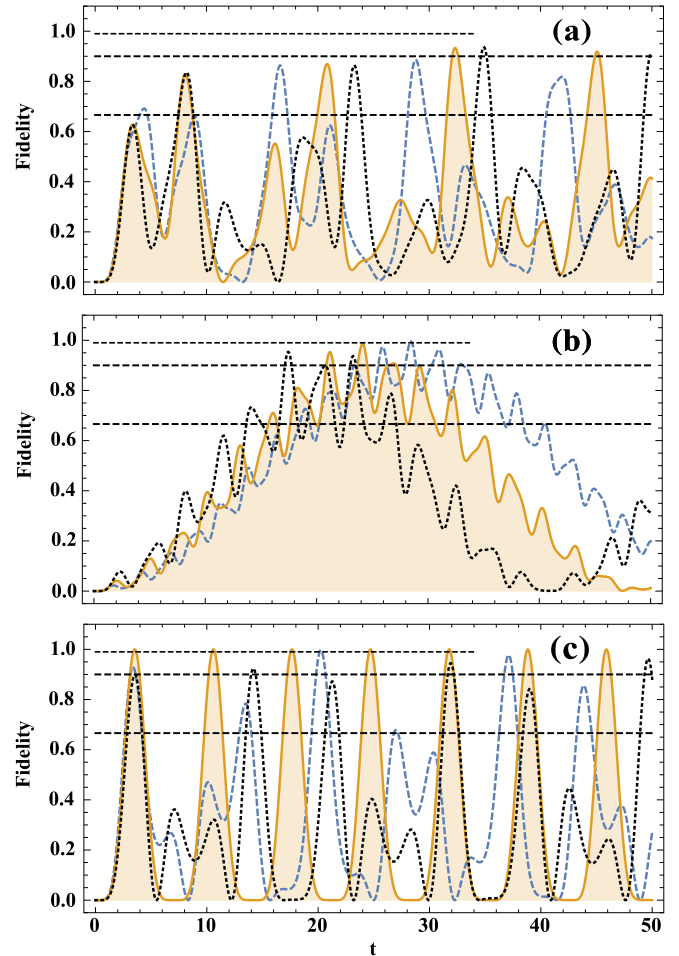


FIG. 3. (Color online) Fidelity $F(t)$ of state transfer in a four-spin system with (a) $\kappa \rightarrow \infty$ (fermions), (b) $\kappa = \frac{1}{2}$, and (c) $\kappa = 2$ [cf. Figs. 2(a), 2(b), and 2(c)], for $u = 0$ (dashed, blue), u_p (solid, orange), and $2u_p$ (dotted, black). For visual aid, the values of $F = 2/3, 0.9, 0.99$ are marked with thin dashed horizontal lines. Time is in units of \hbar/ε .

to the incommensurate spectrum, the fermionic (XXX) case $\kappa \rightarrow \infty$ without external magnetic field (see below) cannot realize perfect state transfer for any u . This we prove in Appendix B, where we also show that bosons with $\kappa = 1$ yield the same fidelity as the fermions in Fig. 3(a). In the bosonic case with $\kappa < 1$, we observe in Fig. 3(b) a slow (third order in J_j) transition between the degenerate initial $|\downarrow\uparrow\uparrow\uparrow\rangle$ and final $|\uparrow\uparrow\uparrow\downarrow\rangle$ states via the nonresonant intermediate states $|\uparrow\downarrow\uparrow\uparrow\rangle$ and $|\uparrow\uparrow\downarrow\uparrow\rangle$ (see Appendix B 2 for details). Finally, the perfect, optimal state transfer is realized in the $\kappa = 2$ (XX) case with $u = u_p$ [Fig. 3(c)], as expected,

We note, finally, that the XXX Hamiltonian can in principle be modified by a spatially inhomogeneous (effective) magnetic field $B(x)\sigma_z$, resulting in

$$\tilde{H}_s = H_s + \sum_{j=1}^N h_j \sigma_z^j, \quad (12)$$

as shown in Appendix C. Then, for $N_\downarrow = 1$, an appropriate choice of the local fields, $h_{1,N} = J_{1,N-1}$ and $h_{j=2,\dots,N-1} = J_{j-1} + J_j$, will equalize the diagonal elements of \tilde{H}_s , turning it into the XX Hamiltonian, which, with proper interspin coupling coefficients J_j determined by the trapping potential $V(x)$, can realize perfect state transfer.

V. CONCLUSIONS

We have shown that a two-component system of strongly interacting atoms in a 1D trap can be represented as a spin chain described by the XXZ model Hamiltonian. Quite generally, any number of atoms N in an arbitrary trapping potential—not necessary spatially periodic—is amenable to such a representation. To obtain the corresponding spin-chain Hamiltonian (7), one has to construct the Slater determinant wave function Φ_0 from N single-particle eigenfunctions in the trap of a given form $V(x)$ and then calculate the overlap integrals

α_j of Eq. (6), yielding the spin-spin interaction coefficients $J_j = -\alpha_j/g$. In turn, the shape of the trapping potential determines the parameters of the resulting Hamiltonian, which permits (reverse) engineering of the desired many-body states and dynamics of the effective spin chain.

Our formalism, while applicable to particles with strong contact interactions, scales favorably with the particle number N . Moreover, our approach is easily extendable to multicomponent (spin $s > 1/2$) systems analogous to spin-chain models with $SU(2s+1)$ symmetry. Chains of coupled qudits of dimension $2s+1 > 2$ exhibit a higher quality of entanglement transfer [37].

The experimental context of our study is cold alkali-metal atoms, e.g., Rb or Li, in small traps of dimension $L \sim 1 \mu\text{m}$, realized by far-detuned focused laser beams or optical lattices. The corresponding energy scale is then $\varepsilon/\hbar \sim 1\text{--}10$ kHz, while strong interactions $g \gg 1$ occur near Feshbach resonances in external magnetic fields. Tailoring magnetic fields on the scale of L could be difficult. Instead, appropriately detuned, tightly focused laser beams can mimic spatially inhomogeneous magnetic fields through differential Stark shifts of the hyperfine (Zeeman) atomic levels and can induce Raman transitions between (spin) states of individual atoms to prepare, initialize, and read out the state of the system as required [7,8].

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APPENDIX A: PERTURBATIVE DERIVATION OF THE ENERGY EIGENVALUES, EQ. (5)

Here we outline the derivation of the energy eigenvalues of Hamiltonian (1). The corresponding eigenvalue problem is defined by the Schrödinger equation

$$\sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^{N_\sigma} h(x_{\sigma,i}) \Psi = E \Psi, \quad (A1)$$

supplemented with the boundary conditions at the contact positions of any two particles,

$$\left(\frac{\partial \Psi}{\partial x_{\sigma,i}} - \frac{\partial \Psi}{\partial x_{\sigma',i'}} \right) \Big|_{x_{\sigma,i} - x_{\sigma',i'} = 0^-}^{x_{\sigma,i} - x_{\sigma',i'} = 0^+} = 2g_{\sigma\sigma'} \Psi(x_{\sigma,i} = x_{\sigma',i'}). \quad (A2)$$

The dependence of the energy E on the interaction strength g can be inferred from the Hellmann-Feynman theorem [31,33], Eq. (4),

$$\frac{\partial E}{\partial g} = \kappa \sum_{\sigma=\uparrow,\downarrow} \sum_{i=1}^{N_\sigma} \sum_{i'=i}^{N_\sigma} \langle \Psi | \delta(x_{\sigma,i} - x_{\sigma,i'}) | \Psi \rangle + \sum_{i=1}^{N_\uparrow} \sum_{i'=1}^{N_\downarrow} \langle \Psi | \delta(x_{\uparrow,i} - x_{\downarrow,i'}) | \Psi \rangle. \quad (A3)$$

Combining Eqs. (A2) and (A3), we obtain for small $1/g$

$$\frac{\partial E}{\partial g} = \frac{K_{\uparrow\downarrow}}{g^2} + \frac{K_{\uparrow\uparrow}}{\kappa g^2} + \frac{K_{\downarrow\downarrow}}{\kappa g^2} + O(1/g^2), \quad (A4)$$

with the interaction parameters $K_{\sigma\sigma'}$ given by

$$K_{\uparrow\downarrow} = \lim_{g \rightarrow \infty} \frac{\sum_{i=1}^{N_\uparrow} \sum_{i'=1}^{N_\downarrow} \int \prod_{j=1}^{N_\uparrow} dx_{\uparrow,j} \prod_{j'=1}^{N_\downarrow} dx_{\downarrow,j'} \left| \left(\frac{\partial \Psi}{\partial x_{\downarrow,i}} - \frac{\partial \Psi}{\partial x_{\uparrow,i'}} \right) \Big|_{x_{\downarrow,i}=x_{\uparrow,i'}=0^+} \right|^2 \delta(x_{\downarrow,i} - x_{\uparrow,i'})}{4 \int \prod_{i=1}^{N_\uparrow} dx_{\uparrow,i} \prod_{i'=1}^{N_\downarrow} dx_{\downarrow,i'} |\Psi|^2}, \quad (\text{A5})$$

$$K_{\sigma\sigma} = \lim_{g \rightarrow \infty} \frac{\sum_{i=1}^{N_\sigma} \sum_{i'=1}^{N_\sigma} \int \prod_{j=1}^{N_\uparrow} dx_{\uparrow,j} \prod_{j'=1}^{N_\downarrow} dx_{\downarrow,j'} \left| \left(\frac{\partial \Psi}{\partial x_{\sigma,i}} - \frac{\partial \Psi}{\partial x_{\sigma,i'}} \right) \Big|_{x_{\sigma,i}=x_{\sigma,i'}=0^+} \right|^2 \delta(x_{\sigma,i} - x_{\sigma,i'})}{4 \int \prod_{i=1}^{N_\uparrow} dx_{\uparrow,i} \prod_{i'=1}^{N_\downarrow} dx_{\downarrow,i'} |\Psi|^2}, \quad (\text{A6})$$

with $\sigma = \uparrow$ or \downarrow . Apparently, different wave functions Ψ with the corresponding combinations of a_k in Eq. (3) lead to different values of $K_{\sigma\sigma'}$, which lifts the degeneracy of the spectrum. By integrating Eq. (A4) with respect to g , we obtain the perturbative expansion (5) used in Sec. II.

APPENDIX B: STATIC AND DYNAMIC PROPERTIES OF THE EFFECTIVE SPIN MODEL WITH $N_\downarrow = 1$ AND $N_\uparrow = 3$

Here we present analytic expressions for the eigenvalues and eigenvectors of the spin Hamiltonian H_s for four particles, three of which are in one internal state (spin up) and the other one is in a different internal state (spin down), and analyze the state transfer dynamics.

In the basis of $\{|\downarrow\uparrow\uparrow\uparrow\rangle, |\uparrow\downarrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\uparrow\downarrow\rangle\}$, the Hamiltonian in Eq. (7) can be cast in the matrix form,

$$H_s - E_0 \mathbf{I} = \begin{pmatrix} J_1 + \frac{2J_1}{\kappa} + \frac{2J_2}{\kappa} & -J_1 & 0 & 0 \\ -J_1 & J_1 + \frac{2J_1}{\kappa} + J_2 & -J_2 & 0 \\ 0 & -J_2 & J_1 + \frac{2J_1}{\kappa} + J_2 & -J_1 \\ 0 & 0 & -J_1 & J_1 + \frac{2J_1}{\kappa} + \frac{2J_2}{\kappa} \end{pmatrix}, \quad (\text{B1})$$

where the $E_0 \mathbf{I}$ term yields a trivial common energy shift for all spin configurations and can therefore be dropped. For finite κ , Eq. (B1) describes bosons, and we see that for $\kappa = 2$ all the diagonal elements of the matrix are the same, which is in fact the Heisenberg XX model. The fermionic limit $\kappa \rightarrow \infty$ corresponds to the isotropic XXX model.

The eigenvalues of Eq. (B1) are

$$\lambda_1 = \frac{2J_1 + \kappa J_1 + J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa}, \quad \lambda_2 = \frac{2J_1 + \kappa J_1 + J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa},$$

$$\lambda_3 = \frac{2J_1 + \kappa J_1 + J_2 + \kappa J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + \kappa^2 J_2^2}}{\kappa}, \quad \lambda_4 = \frac{2J_1 + \kappa J_1 + J_2 + \kappa J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + \kappa^2 J_2^2}}{\kappa},$$

with the corresponding (non-normalized) eigenvectors

$$|\Psi_1\rangle = \left\{ 1, \frac{J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa J_1}, \frac{J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa J_1}, 1 \right\},$$

$$|\Psi_2\rangle = \left\{ 1, \frac{J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa J_1}, \frac{J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa J_1}, 1 \right\},$$

$$|\Psi_3\rangle = \left\{ -1, -\frac{J_2 - \kappa J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + \kappa^2 J_2^2}}{\kappa J_1}, \frac{J_2 - \kappa J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + \kappa^2 J_2^2}}{\kappa J_1}, 1 \right\},$$

$$|\Psi_4\rangle = \left\{ -1, -\frac{J_2 - \kappa J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + \kappa^2 J_2^2}}{\kappa J_1}, \frac{J_2 - \kappa J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + \kappa^2 J_2^2}}{\kappa J_1}, 1 \right\}.$$

1. Fermions

In the limit of $\kappa \rightarrow \infty$, the ordered eigenvalues and normalized eigenvectors reduce to

$$\lambda_1^{(f)} = 0, \quad |\Psi_1^{(f)}\rangle = \frac{1}{2} \{1, 1, 1, 1\}; \quad \lambda_2^{(f)} = J_1 + J_2 - \sqrt{J_1^2 + J_2^2},$$

$$|\Psi_2^{(f)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 - J_2\sqrt{J_1^2 + J_2^2}}} \{-J_1, J_2 - \sqrt{J_1^2 + J_2^2}, -J_2 + \sqrt{J_1^2 + J_2^2}, J_1\};$$

$$\lambda_3^{(f)} = 2J_1, \quad |\Psi_3^{(f)}\rangle = \frac{1}{2}\{1, -1, -1, 1\}; \quad \lambda_4^{(f)} = J_1 + J_2 + \sqrt{J_1^2 + J_2^2},$$

$$|\Psi_4^{(f)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 + J_2\sqrt{J_1^2 + J_2^2}}}\{-J_1, J_2 + \sqrt{J_1^2 + J_2^2}, -J_2 - \sqrt{J_1^2 + J_2^2}, J_1\}.$$

Our aim is to transfer the initial state $|\Psi_{\text{in}}^{(f)}\rangle = |\downarrow\uparrow\uparrow\uparrow\rangle$, which evolves in time as

$$|\Psi^{(f)}(t)\rangle = \frac{1}{2}|\Psi_1^{(f)}\rangle e^{-i\lambda_1^{(f)}t} - \frac{J_1}{2\sqrt{J_1^2 + J_2^2 - J_2\sqrt{J_1^2 + J_2^2}}}|\Psi_2^{(f)}\rangle e^{-i\lambda_2^{(f)}t} + \frac{1}{2}|\Psi_3^{(f)}\rangle e^{-i\lambda_3^{(f)}t} - \frac{J_1}{2\sqrt{J_1^2 + J_2^2 + J_2\sqrt{J_1^2 + J_2^2}}}|\Psi_4^{(f)}\rangle e^{-i\lambda_4^{(f)}t},$$

to the final state

$$|\Psi_{\text{out}}^{(f)}\rangle = |\uparrow\uparrow\uparrow\downarrow\rangle = \frac{1}{2}|\Psi_1^{(f)}\rangle + \frac{J_1}{2\sqrt{J_1^2 + J_2^2 - J_2\sqrt{J_1^2 + J_2^2}}}|\Psi_2^{(f)}\rangle + \frac{1}{2}|\Psi_3^{(f)}\rangle + \frac{J_1}{2\sqrt{J_1^2 + J_2^2 + J_2\sqrt{J_1^2 + J_2^2}}}|\Psi_4^{(f)}\rangle.$$

The necessary and sufficient conditions for this are

$$(\lambda_{n+1}^{(f)} - \lambda_n^{(f)})t_{\text{out}} = (2m_n + 1)\pi, \quad (\text{B2})$$

where m_n are some positive integers and t_{out} is a transfer time. This leads to two equations for $m_{1,2,3}$:

$$\frac{1 - r + \sqrt{1 + r^2}}{1 + r - \sqrt{1 + r^2}} = \frac{2m_2 + 1}{2m_1 + 1}, \quad \frac{-1 + r + \sqrt{1 + r^2}}{1 + r - \sqrt{1 + r^2}} = \frac{2m_3 + 1}{2m_1 + 1},$$

which determine the ratio $r = J_2/J_1$ for perfect state transfer. These equations can only be satisfied if

$$2m_1 = -2 - m_2 - m_3 + \sqrt{2 + 4m_2 + m_2^2 + 4m_3 + 6m_2m_3 + m_3^2} \quad \text{or} \quad (\text{B3})$$

$$2m_1 = m_2 + m_3 + \sqrt{2 + 4m_2 + m_2^2 + 4m_3 + 6m_2m_3 + m_3^2}.$$

Since m_1 is an integer, $\sqrt{2 + 4m_2 + m_2^2 + 4m_3 + 6m_2m_3 + m_3^2} = k$ should also be some integer k . First notice that

$$2 + 4m_2 + m_2^2 + 4m_3 + 6m_2m_3 + m_3^2 = 2(m_2 + m_3 + 1)^2 - (m_2 - m_3)^2.$$

We now prove that the condition

$$k^2 + (m_2 - m_3)^2 = 2(m_2 + m_3 + 1)^2 \quad (\text{B4})$$

cannot be satisfied with any set of integers m_2, m_3 and k . There are four possible cases: (i) k is odd and $(m_2 - m_3)$ is even, (ii) k is even and $(m_2 - m_3)$ is odd, (iii) both k and $(m_2 - m_3)$ are odd, and (iv) both k and $(m_2 - m_3)$ are even. Note that if $(m_2 - m_3)$ is odd (even), then $(m_2 + m_3 + 1)$ is even (odd). Cases (i) and (ii) are then ruled out since they yield an odd left-hand side (lhs) of Eq. (B4), whereas the right-hand side (rhs) is always even. For case (iii) the rhs is divisible by 4 without a remainder and the lhs is not. Finally, for case (iv) the lhs is divisible by 4 without a remainder and the rhs is not. This means that conditions (B3) cannot be satisfied. Hence, an isotropic (XXX) spin chain cannot realize perfect state transfer, unless the diagonal elements of the Hamiltonian matrix in Eq. (B1) are modified by a local (magnetic field) perturbation, cf. Eq. (C4) below.

2. Bosons

We now consider bosons with $\kappa = 1$, leading to the following eigenvalues and eigenvectors:

$$\lambda_1^{(b)} = 3J_1 + J_2 - \sqrt{J_1^2 + J_2^2}, \quad |\Psi_1^{(b)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 + J_2\sqrt{J_1^2 + J_2^2}}}\{J_1, J_2 + \sqrt{J_1^2 + J_2^2}, J_2 + \sqrt{J_1^2 + J_2^2}, J_1\};$$

$$\lambda_2^{(b)} = 2J_1 + 2J_2, \quad |\Psi_2^{(b)}\rangle = \frac{1}{2}\{-1, -1, 1, 1\};$$

$$\lambda_3^{(b)} = 3J_1 + J_2 + \sqrt{J_1^2 + J_2^2}, \quad |\Psi_3^{(b)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 - J_2\sqrt{J_1^2 + J_2^2}}}\{J_1, J_2 - \sqrt{J_1^2 + J_2^2}, J_2 - \sqrt{J_1^2 + J_2^2}, J_1\};$$

$$\lambda_4^{(b)} = 4J_1 + 2J_2, \quad |\Psi_4^{(b)}\rangle = \frac{1}{2}\{-1, 1, -1, 1\}.$$

The initial state $|\Psi_{\text{in}}^{(b)}\rangle = |\downarrow\uparrow\uparrow\uparrow\rangle$ now evolves as

$$|\Psi^{(b)}(t)\rangle = \frac{J_1}{2\sqrt{J_1^2 + J_2^2 + J_2\sqrt{J_1^2 + J_2^2}}} |\Psi_1^{(b)}\rangle e^{-i\lambda_1^{(b)}t} - \frac{1}{2} |\Psi_2^{(b)}\rangle e^{-i\lambda_2^{(b)}t} \\ + \frac{J_1}{2\sqrt{J_1^2 + J_2^2 - J_2\sqrt{J_1^2 + J_2^2}}} |\Psi_3^{(b)}\rangle e^{-i\lambda_3^{(b)}t} - \frac{1}{2} |\Psi_4^{(b)}\rangle e^{-i\lambda_4^{(b)}t}.$$

Note that $\lambda_4^{(b)} - \lambda_3^{(b)} = \lambda_2^{(f)}$, $\lambda_4^{(b)} - \lambda_2^{(b)} = \lambda_3^{(f)}$, and $\lambda_4^{(b)} - \lambda_1^{(b)} = \lambda_4^{(f)}$. As a result, the fidelity of state transfer, $F(t) \equiv |\langle\Psi(t)|\uparrow\uparrow\uparrow\downarrow\rangle|^2$, is the same for both fermions ($\kappa \rightarrow \infty$) and bosons with $\kappa = 1$, which holds true for $N_\downarrow = 1$ and any N_\uparrow .

Next, in the special case of perfect state transfer, $J_2/J_1 = \sqrt{4/3}$, with the Heisenberg XX model, $\kappa = 2$, we have the equidistant spectrum $\lambda_1^{(b)} = \frac{\sqrt{12}-1}{2}J_2$, $\lambda_2^{(b)} = \lambda_1^{(b)} + J_2$, $\lambda_3^{(b)} = \lambda_1^{(b)} + 2J_2$, and $\lambda_4^{(b)} = \lambda_1^{(b)} + 3J_2$, leading to the fastest transfer time $t_{\text{out}} = \pi/J_2$.

The final case discussed in the text concerns the limit $\kappa \ll 1$ when interspecies interaction is much larger than the intraspecies interaction. Then the two lowest eigenstates $|\Psi_1^{(b)}\rangle \simeq \frac{1}{\sqrt{2}}\{1,0,0,1\}$ and $|\Psi_2^{(b)}\rangle \simeq \frac{1}{\sqrt{2}}\{-1,0,0,1\}$ become degenerate, $\lambda_1^{(b)} \simeq \lambda_2^{(b)}$ and separated from the other two eigenstates $|\Psi_3^{(b)}\rangle \simeq \frac{1}{\sqrt{2}}\{0,1,1,0\}$ and $|\Psi_4^{(b)}\rangle \simeq \frac{1}{\sqrt{2}}\{0,-1,1,0\}$ by $\lambda_{3,4}^{(b)} - \lambda_1^{(b)} \simeq \frac{2J_2}{\kappa} \pm J_2$. The state transfer between the initial $|\downarrow\uparrow\uparrow\uparrow\rangle$ and final $|\uparrow\uparrow\uparrow\downarrow\rangle$ states proceeds then via nonresonant intermediate states $|\uparrow\downarrow\uparrow\uparrow\rangle$ and $|\uparrow\uparrow\downarrow\uparrow\rangle$ as a third-order process with the effective Rabi frequency $J_{\text{eff}} \simeq \frac{J_1 J_2 J_1}{(2J_2/\kappa)^2} = \frac{\kappa^2 J_1^2}{4J_2}$.

APPENDIX C: EFFECTIVE SPIN MODEL IN A MAGNETIC FIELD

Here we outline the derivation of the effective spin Hamiltonian \tilde{H}_s for N particles in an (effective) external magnetic field $B(x)\sigma_z$. We consider a single spin-down particle $N_\downarrow = 1$ and assume a weak magnetic field $B(x) = b(x)/g$ ($g \gg 1$) which modifies the Hamiltonian H of Eq. (1) as

$$\tilde{H} = H + \sum_{i=1}^{N-1} \frac{b(x_{\uparrow,i})}{g} - \frac{b(x_{\downarrow,1})}{g}. \quad (\text{C1})$$

For the corresponding energy of N -particle eigenfunction Ψ , to linear order in $1/g$, we then obtain

$$\tilde{E} = E - 2 \frac{\sum_{j=1}^N \frac{\beta_j a_j^2}{g}}{\sum_{j=1}^N a_j^2} + \sum_{j=1}^N \beta_j, \quad (\text{C2})$$

where we write simply a_j instead of $a_{j|k}$ for a single impurity (spin-down) particle, while the geometric factors are

$$\beta_j = \frac{\int \prod_{i=1}^{N-1} dx_{\uparrow,i} dx_{\downarrow,1} |\Phi_0|^2 b(x_{\downarrow,1})}{\int \prod_{i=1}^{N-1} dx_{\uparrow,i} dx_{\downarrow,1} |\Phi_0(\{x_{\uparrow,i}, x_{\downarrow,1}\})|^2}, \quad (\text{C3})$$

where in Φ_0 in the numerator the spin-down particle $x_{\downarrow,1}$ is placed at position j . The effective spin Hamiltonian for the case $\kappa \rightarrow \infty$ can now be cast as

$$\tilde{H}_s = E_0 \mathbf{I} - \frac{1}{2} \sum_{j=1}^{N-1} J_j (\sigma^j \sigma^{j+1} - \mathbf{I}) + \sum_{j=1}^N h_j \sigma_z^j, \quad (\text{C4})$$

with $h_j = \beta_j$.

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