Engineering the Dynamics of Effective Spin-Chain Models for Strongly Interacting Atomic Gases

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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 tuning independently the parameters of the spin Hamiltonian through interatomic (intra-species) 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 non-trivial system of four particles representing exchange-coupled qubits.

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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 single atom per lattice site has been demonstrated [11,12]. The Mott-Hubbard insulator for a two-component system can be mapped onto the Heisenberg spin Hamiltonian [13,14] facilitating studies of interacting spin models responsible for many key features of quantum magnetism [15]. 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 show that a 1D ensemble of strongly-interacting atoms with any external confinement can, quite generally, be represented as a spin-chain. 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 and quantum statistics of the constituent atoms (bosons or fermions). This opens several possibilities for engineering desired stationary and dynamic quantum states. As a revealing example amenable to analytic treatment, we consider the problem of quantum state transfer [26–28] in the simplest yet non-trivial case of four particles. We find that by optimal choice of the trapping potential and intra-species interactions between bosonic atoms, perfect state transfer [26–28] 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 \( N \)-atom system. 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

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

where \( h(x) = -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + \frac{\hbar^2}{mL^2} V(x/L) \) is the single particle Hamiltonian, \( m \) is the mass assumed equal for all particles, and \( x_{\sigma,i} \) 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 \( g_{\uparrow\downarrow} \equiv g \geq 0 \) and \( g_{\downarrow\downarrow} \equiv g_{\uparrow\uparrow} \equiv \kappa g \).
with \( \kappa > 0 \). Hamiltonian (11) 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 wavefunctions \( \Psi(P_0) \{ \{ x_{\uparrow,1}, x_{\downarrow,1} \} \} \) for various configurations \( \{ x_{\uparrow,1}, x_{\downarrow,1} \} \) of atomic positions. There are in fact \( \binom{N}{N_1} = \frac{N!}{N_1!N_{\uparrow,1}!N_{\downarrow,1}!} \) distinguishable configurations with different ordering of atoms, e.g., \( x_{\uparrow,1} < x_{\uparrow,2} < x_{\downarrow,1} < \ldots < x_{\uparrow,N} < \ldots < x_{\downarrow,1} \). In the limit of \( 1/g \to 0 \), the requirement of finite energy implies that \( \Psi \) should vanish whenever the coordinates of any two particles coincide, \( x_{\uparrow,1} = x_{\downarrow,1} \). This requirement can only be satisfied by the Slater determinant wavefunction for \( N \) particles, which is completely antisymmetric superposition of the products of different single-particle wavefunctions representing solutions of the single particle Hamiltonian \( h(x) \).

Consider the Slater determinant wavefunction \( \Psi_0 \) composed of the \( N \) lowest-energy single-particle eigenfunctions of \( h(x) \). For \( 1/g \to 0 \), all \( M(N_{\uparrow},N_{\downarrow}) = \binom{N_{\uparrow}+N_{\downarrow}}{N_{\uparrow}} \) configurations of atomic coordinates yield the same energy \( E_0 \) for \( \Psi_0 \{ \{ x_{\uparrow,1}, x_{\downarrow,1} \} \} \). For small but finite \( 1/g \), the degeneracy of this ground state manifold is lifted. We can expand the general \( N \)-particle eigenfunction as

\[
\Phi = \sum_{k=1}^{M(N_{\uparrow},N_{\downarrow})} a_k \Pi_k \Psi_0 \{ \{ x_{\uparrow,1}, x_{\downarrow,1} \} \},
\]

where \( \{ x_{\uparrow,1}, x_{\downarrow,1} \} \equiv x_{\uparrow,1} < \ldots < x_{\uparrow,N_{\uparrow}} < x_{\downarrow,1} < \ldots < x_{\downarrow,N_{\downarrow}} \) and the sum is over all the permutations \( \Pi_k \) of coordinates. Using the perturbative approach of Ref. [30], the corresponding energy, to linear order in \( 1/g \), is obtained as

\[
E = E_0 - \frac{1}{2} \sum_{j=1}^{N-1} \frac{a_j}{\sum_{k=1}^{M(N_{\uparrow},N_{\downarrow})} a_k^2} \left( A_j + \frac{2}{3} C_j + \frac{2}{3} D_j \right),
\]

where \( A_j = \sum_{k=1}^{M(N_{\uparrow}-1,N_{\downarrow}-1)} (a_{jk} - b_{jk})^2 \), while \( C_j = \sum_{k=1}^{M(N_{\uparrow}-2,N_{\downarrow}-2)} c_{jk}^2 \) and \( D_j = \sum_{k=1}^{M(N_{\uparrow}-2,N_{\downarrow})} d_{jk}^2 \) for bosons and \( C_j = D_j = 0 \) for fermions. Here \( a_{jk} \) denote the coefficients in the expansion (2) multiplying terms \( \Psi_0(\ldots < x_{\uparrow} < x_{\downarrow} \ldots) \) with \( x_{\uparrow} \) at position \( j \) followed by \( x_{\downarrow} \) at position \( j+1 \), while \( b_{jk} \) are the coefficients of \( \Psi_0(\ldots < x_{\downarrow} < x_{\uparrow} \ldots) \) with \( x_{\uparrow} \) and \( x_{\downarrow} \) swapped. Likewise, for identical bosons, \( c_{jk} \) denote the expansion coefficients in Eq. (2) in front of \( \Psi_0(\ldots < x_{\uparrow} < x_{\downarrow} \ldots) \) with \( x_{\uparrow} \) at position \( j \) followed by \( x_{\downarrow} \) at position \( j+1 \), while \( d_{jk} \) are the coefficients of \( \Psi_0(\ldots < x_{\downarrow} < x_{\uparrow} \ldots) \) with \( x_{\uparrow} \) and \( x_{\downarrow} \) swapped.

Finally, the geometric factors \( a_j \) are solely determined by the confining potential through \( \Psi_0 \) as

\[
\alpha_j = \frac{\int \prod_{i=1}^{N_{\uparrow}} dx_{\uparrow,i} \prod_{i=1}^{N_{\downarrow}} dx_{\downarrow,i} \left( \frac{\partial \Psi_0}{\partial x_{\uparrow,i}} \right)^2 \delta(x_{\uparrow,j} - x_{\uparrow,1})}{\frac{\int \prod_{i=1}^{N_{\uparrow}} dx_{\uparrow,i} \prod_{i=1}^{N_{\downarrow}} dx_{\downarrow,i} |\Psi_0(\{x_{\uparrow,i}, x_{\downarrow,i}\})|^2},
\]

where in \( \Psi_0 \) in the numerator the spin-down atom \( x_{\downarrow,1} \) is placed at position \( j+1 \) following \( j \) spin-up atoms \( x_{\uparrow,1}, \ldots, x_{\uparrow,j} \). Below we deal mostly with bosons as they can also reproduce fermions in the limit of \( \kappa \to \infty \).

The effective spin-chain model. We now demonstrate that Hamiltonian (11) for \( N = N_{\uparrow} + N_{\downarrow} \) strongly-interacting particles, \( 1/g \ll 1 \), can be mapped onto the spin-\( \frac{1}{2} \) XXX Hamiltonian of the form

\[
H_s = E_0 I - \frac{1}{2} \sum_{j=1}^{N-1} \left[ J_j (\sigma^j \sigma^{j+1} - I) - \frac{2J_z}{\kappa} (\sigma_z^j \sigma_{\uparrow}^{j+1} + I) \right],
\]

where \( I \) is the identity matrix, \( \sigma^j = (\sigma_z^j, \sigma_\uparrow^j, \sigma_\downarrow^j) \) 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 (5) can be expanded in terms of the spin permutations \( \Pi_k \) as

\[
|\Phi\rangle = \sum_{k=1}^{M(N_{\uparrow},N_{\downarrow})} a_k \Pi_k |\uparrow_1 \ldots \uparrow_{N_{\uparrow}} \downarrow_1 \ldots \downarrow_{N_{\downarrow}}\rangle.
\]

Consider the energy expectation value \( \langle\Phi|H_s|\Phi\rangle \). Using the swap operator \( P_{j,j+1} = \frac{1}{2} (\sigma^j \sigma^{j+1} + I) \), we find that non-zero contributions to \( \langle\Phi|H_s|\Phi\rangle \) are \( |a_{jk}| \langle \Psi_{jk}|P_{j,j+1}|\Psi_{jk}\rangle \) or \( b_{jk}|\Psi_{jk}|b_{jk}|\Psi_{jk}\rangle \) and \( c_{jk}|\Psi_{jk}|b_{jk}|\Psi_{jk}\rangle \) or \( d_{jk}|\Psi_{jk}|b_{jk}|\Psi_{jk}\rangle \), where \( |\Psi_{jk}\rangle \equiv |\ldots \uparrow_j \downarrow_{j+1} \ldots\rangle \). Assuming normalization \( \langle\Phi|\Phi\rangle = 1 \), we then obtain

\[
\langle\Phi|H_s|\Phi\rangle = E_0 + \sum_{j=1}^{N-1} \left( A_j + \frac{2}{3} C_j + \frac{2}{3} D_j \right),
\]

with \( A_j, C_j \) and \( D_j \) having the same meaning as above. Comparison of Eqs. (3) and (7) reveals that, to linear order in \( 1/g \), the eigenvalue problem for Hamiltonians (11) and (5) is the same, with the corresponding spin-spin interaction coefficients given by \( J_j = -\alpha_j/g \). Note that for fermions or hard-core bosons, \( \kappa \to \infty \), Eq. (5) becomes the XXX Hamiltonian, while in the special case of bosons with \( \kappa = 2 \), it reduces to the XX model Hamiltonian. These results are summarized in Table 1.

For concreteness, we have contemplated so far only the ground state energy manifold of Hamiltonian (11). Yet, precisely the same arguments apply to any \( n \)th excited state manifold which can be represented by a corresponding XXX Hamiltonian (5) disconnected from all the other energy manifolds, each located in the vicinity of energy \( E_n \) of the corresponding Slater determinant wavefunction \( \Psi_n \).
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. (5), through the trapping potential $V(x)$ and interparticle interactions $g \gg 1$ and $\kappa > 0$. As an illustration, consider a relatively simple yet non-trivial system of four particles confined in a symmetric 1D trap of the form (see Fig. 1)

$$V(x) = -V_0 \sin^2 \left[ \frac{1}{2} (x + 1) \pi \right] - u \sin^2 [(x + 1) \pi], \quad (8)$$

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 wavefunctions $\Psi_0$.

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 non-trivial 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 $\lambda_n$ of $H_s$ and the ratio $J_2/J_1$ on the parameter $u$ of the potential of Eq. (8).

Clearly, for $u \ll V_0$ the potential $V(x)$ is nearly harmonic, leading to larger overlap of the wavefunctions of the particles in the middle of the trap, which results in $J_2/J_1 \simeq 1.4$. 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 non-interacting parts with vanishing coupling $J_2$ in the middle and doubly degenerate eigenvalues. This tendency can be seen in Fig. 2(a)-(c), where we use three representative values of $\kappa$. The fermionic case of $\kappa \rightarrow \infty$ corresponds to isotropic spin Hamiltonian (see also SM [32]). In the bosonic case with $\kappa < 1$, the interaction with the impurity (spin-down) particle is stronger than the interaction between identical (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, which was also discussed in [32] (see also the SM [32]). 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).

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 [23, 28]. 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

![FIG. 1: (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. (5) for $V_0 = 50\varepsilon$ and $u = (0, 1, 2, 4) \times u_p$ (top to bottom) with $u_p \simeq 12.5\varepsilon$.](image)

![FIG. 2: Energy eigenvalues $\lambda_n$ of $H_s$ (less the $E_0I$ term) vs $u$ of Eq. (8), for $N_1 = 1$, $N_1 = 3$ and (a) $\kappa \rightarrow \infty$ (fermions), (b) $\kappa = \frac{2}{3}$, 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 equidistant spectrum in (c). $\lambda$'s and $u$ are in units of $\varepsilon$ and $g = 100$.](image)

| Spin-$\frac{1}{2}$ model | Constituents          | $\kappa$ |
|------------------------|-----------------------|----------|
| $XXZ$                  | bosons                | $0 < \kappa < \infty$ |
| $XXX$                  | bosons or fermions    | $\kappa \rightarrow \infty$ |
| $XX$                   | bosons                | $\kappa = 2$ |
tunable spin chains \[34\].

In its standard form \[23, 24, 34\], the quantum state transfer protocol involves preparing the spin chain in a dynamically passive state, e.g., \(|↑↑\ldots↑⟩\), and then initializing at time \(t_{\text{in}} = 0\) the first spin with the qubit state \(|ψ⟩ = α|↑⟩ + β|↓⟩\) to be transferred. Ideal transfer would imply that at a well-defined time \(t_{\text{out}}\) the last spin of the chain is in state \(|ψ⟩\) (up to a certain relative phase \(ϕ_0\) between the amplitudes of \(|↑⟩\) and \(|↓⟩\)). Since for the qubit state \(|↑⟩\) the spin chain remains in the passive state, our aim is to maximize the probability of attaining state \(|↑↑\ldots↑⟩\) at time \(t_{\text{out}}\) given that at time \(t = 0\) its state was \(|ψ(0)⟩ = |↓\ldots↓⟩\). We thus define the fidelity of state transfer as

\[
F(t) \equiv |⟨ψ(t)|↑↑\ldots↑⟩|^2. \tag{9}
\]

The chain of four spins initialized as shown in Fig. (a) represents the smallest non-trivial system in which achieving perfect state transfer, \(F(t_{\text{out}}) = 1\), requires judicious choice of the parameters of Hamiltonian \(H\). \[33\]. The necessary and sufficient condition is a commensurate spectrum of \(H\), \[28\], namely \(e^{-i\hat{H}t_{\text{out}}/\hbar} = (-1)^n e^{iϕ}\) with some \(ϕ\), the equidistant spectrum, \(λ_{n+1} - λ_n = Δλ\forall n\), being optimal \[36\] in terms of the fastest transfer time \(t_{\text{out}} = h\pi/Δλ\). In the case of the \(XX\) Hamiltonian, perfect and optimal state transfer is realized by choosing the coupling constants as \(J_j = J_0(\sqrt{(N - j)})\) \[26, 27\] resulting in \(t_{\text{out}} = h\pi/2J_0\). For our system of four spins, this corresponds to \(J_2/J_1 = \sqrt{4/3}\) [see Fig. (c),(d)] and transfer time \(t_{\text{out}} = h\pi/2J_2\).

In Fig. (b) we show the time-dependence of fidelities \(F(t)\) of state transfer for the same values of \(κ\) as in Fig. (a). Due to incommensurate spectrum, the fermionic \((XX)\) case \(κ \to \infty\) without external magnetic field (see below) cannot realize perfect state transfer for any \(u\). This we prove in SM \[32\], where we also show that bosons with \(κ = 1\) yield the same fidelity as fermions in Fig. (a). In the bosonic case with \(κ < 1\), we observe in Fig. (b) a slow (third order in \(J_j\)) transition between the degenerate initial \(|↓\ldots↓⟩\) and final \(|↑↑\ldots↑⟩\) states via nonresonant intermediates states \(|↑↓\ldots\rangle\) and \(|↑↑↑\ldots\rangle\). Finally, the perfect, optimal state transfer is realized in the \(κ = 2\) \((XX)\) case with \(u = u_p\), Fig. (c), as expected.

We note that the XXX Hamiltonian can in principle be modified by a spatially inhomogeneous (effective) magnetic field \(B(x)σ_z\), resulting in \(H_s = H_s + \sum_{j=1}^{N} h_j σ_z\), as shown in SM \[32\]. Then, for \(N_\uparrow = 1\), an appropriate choice of the local fields, \(h_{1,N} = J_1,N^{-1}\) and \(h_{j = 2,...,N-1} = J_{j-1} + J_{j}\), will equalize the diagonal elements of \(H_s\), 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.

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 in an arbitrary trapping potential – not necessary spatially periodic – is amenable to such a representation. 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 \(2s + 1\) exhibit higher quality of entanglement transfer \[37\].

The experimental context of our study is cold alkali atoms, e.g., Rb or Li, in small traps of dimension \(L \sim 1\,\mu m\) realized by far-detuned focused laser beams or optical lattices. The corresponding energy scale is then \(\epsilon/\hbar \sim 1 - 10\,kHz\), 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 [25, 26].

During the preparation of this manuscript, we became aware of a paper by Deuretzbacher et al. [38] which also arrives at a spin model Hamiltonian for two-component systems in a harmonic trap for the case $\kappa \to \infty$.

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SUPPLEMENTAL MATERIAL

Static and dynamic properties of the effective spin model with $N_s = 1$ and $N_f = 3$

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 $\{|\downarrow\uparrow\uparrow\uparrow\rangle, |\downarrow\downarrow\uparrow\uparrow\rangle, |\uparrow\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\uparrow\downarrow\rangle\}$, the Hamiltonian (5) of the main text can be cast in the matrix form

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

where the $E_0 \mathbf{I}$ term yields a trivial common energy shift for all spin configurations and can therefore be dropped. For finite $\kappa$, Eq. (10) 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 $\kappa \to \infty$ corresponds to the isotropic $XXX$ model.

The eigenvalues of Eq. (10) are

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

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

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

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

with the corresponding (non-normalized) eigenvectors

$$|\Phi_1\rangle = \begin{cases} 1, & \frac{J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa J_1}, J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2}, 1, \end{cases},$$

$$|\Phi_2\rangle = \begin{cases} 1, & \frac{J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2}}{\kappa J_1}, J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2}, 1, \end{cases},$$

$$|\Phi_3\rangle = \begin{cases} -1, & \frac{-J_2 - \kappa J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + 2\kappa^2 J_2^2}}{\kappa J_1}, J_2 - \kappa J_2 + \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + 2\kappa^2 J_2^2}, 1, \end{cases},$$

$$|\Phi_4\rangle = \begin{cases} -1, & \frac{-J_2 - \kappa J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + 2\kappa^2 J_2^2}}{\kappa J_1}, J_2 - \kappa J_2 - \sqrt{\kappa^2 J_1^2 + J_2^2 - 2\kappa J_2^2 + 2\kappa^2 J_2^2}, 1, \end{cases}.$$  

**Fermions**

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

$$\lambda_1^{(f)} = 0, \quad |\Phi_1^{(f)}\rangle = \frac{1}{2}(1, 1, 1, 1);$$

$$\lambda_2^{(f)} = J_1 + J_2 - \sqrt{J_1^2 + J_2^2}, \quad |\Phi_2^{(f)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 - J_2 \sqrt{J_1^2 + J_2^2}}}(-J_1, J_2 - \sqrt{J_1^2 + J_2^2}, -J_2 + \sqrt{J_1^2 + J_2^2}, J_1);$$

$$\lambda_3^{(f)} = 2J_1, \quad |\Phi_3^{(f)}\rangle = \frac{1}{2}(1, -1, -1, 1);$$

$$\lambda_4^{(f)} = J_1 + J_2 + \sqrt{J_1^2 + J_2^2}, \quad |\Phi_4^{(f)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 + J_2 \sqrt{J_1^2 + J_2^2}}}(-J_1, J_2 + \sqrt{J_1^2 + J_2^2}, -J_2 - \sqrt{J_1^2 + J_2^2}, J_1).$$
Our aim is to transfer the initial state $|\Psi^{(i)}_{in}\rangle = |↓↑↑\rangle$, which evolves in time as

$$
|\Psi^{(f)}(t)\rangle = \frac{1}{2} |\Phi^{(f)}_1\rangle e^{-i\lambda_1^{(f)} t} - \frac{J_1}{2\sqrt{J_1^2 + J_2^2 - J_2 \sqrt{J_1^2 + J_2^2}}} |\Phi^{(f)}_2\rangle e^{-i\lambda_2^{(f)} t} 
+ \frac{1}{2} |\Phi^{(f)}_3\rangle e^{-i\lambda_3^{(f)} t} - \frac{J_1}{2\sqrt{J_1^2 + J_2^2 + J_2 \sqrt{J_1^2 + J_2^2}}} |\Phi^{(f)}_4\rangle e^{-i\lambda_4^{(f)} t},
$$

to the final state

$$
|\Psi^{(f)}_{out}\rangle = |↑↑↓\rangle = \frac{1}{2} |\Phi^{(f)}_1\rangle + \frac{J_1}{2\sqrt{J_1^2 + J_2^2 - J_2 \sqrt{J_1^2 + J_2^2}}} |\Phi^{(f)}_2\rangle 
+ \frac{1}{2} |\Phi^{(f)}_3\rangle + \frac{J_1}{2\sqrt{J_1^2 + J_2^2 + J_2 \sqrt{J_1^2 + J_2^2}}} |\Phi^{(f)}_4\rangle.
$$

The necessary and sufficient conditions for this are

$$(\lambda_{n+1}^{(f)} - \lambda_n^{(f)}) t_{out} = (2m_n + 1)\pi, \quad (11)$$

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

$$
\frac{1 - r + \sqrt{1 + r^2}}{1 + r - \sqrt{1 + r^2}} = \frac{2m_2 + 1}{2m_1 + 1}, \quad (12)
$$

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

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

or

$$
2m_1 = m_2 + m_3 + \sqrt{2 + 4m_2 + m_2^2 + 4m_3 + 6m_2m_3 + m_3^2}. \quad (13)
$$

Since $m_1$ is integer, $\sqrt{2 + 4m_2 + m_2^2 + 4m_3 + 6m_2m_3 + m_3^2}$ should also be integer. However

$$
\sqrt{2 + 4m_2 + m_2^2 + 4m_3 + 6m_2m_3 + m_3^2} = (m_2 + m_3 + 1) \sqrt{2 - \frac{(m_2 - m_3)^2}{(m_2 + m_3 + 1)^2}}, \quad (13)
$$

and since $\frac{(m_2 - m_3)^2}{(m_2 + m_3 + 1)^2} < 1$, condition (12) cannot be satisfied. Hence, an isotropic (XXX) spin-chain cannot realize a perfect state transfer, unless the diagonal elements of the Hamiltonian matrix in Eq. (10) are modified by local (magnetic field) perturbation, cf. Eq. (16) below.

**Bosons**

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

$$
\lambda_1^{(b)} = 3J_1 + J_2 - \sqrt{J_1^2 + J_2^2}, \quad |\Phi_1^{(b)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 + J_2 \sqrt{J_1^2 + J_2^2}}} (J_1, J_2 + \sqrt{J_1^2 + J_2^2}, J_2 + \sqrt{J_1^2 + J_2^2}, J_1);
$$

$$
\lambda_2^{(b)} = 2J_1 + 2J_2, \quad |\Phi_2^{(b)}\rangle = \frac{1}{2} \{-1, -1, 1, 1\};
$$

$$
\lambda_3^{(b)} = 3J_1 + J_2 + \sqrt{J_1^2 + J_2^2}, \quad |\Phi_3^{(b)}\rangle = \frac{1}{2\sqrt{J_1^2 + J_2^2 - J_2 \sqrt{J_1^2 + J_2^2}}} (J_1, J_2 - \sqrt{J_1^2 + J_2^2}, J_2 - \sqrt{J_1^2 + J_2^2}, J_1);
$$

$$
\lambda_4^{(b)} = 4J_1 + 2J_2, \quad |\Phi_4^{(b)}\rangle = \frac{1}{2} \{-1, 1, -1, 1\}.\quad (16)
$$
The initial state $|\Psi_{\text{in}}^{(b)}\rangle = |\downarrow\uparrow\uparrow\uparrow\rangle$ now evolves as

$$
|\Psi^{(b)}(t)\rangle = \frac{J_1}{2\sqrt{J_1^2 + J_2^2 + J_2\sqrt{J_1^2 + J_2^2}}} |\Phi_1^{(b)}\rangle e^{-i\lambda_1^{(b)} t} - \frac{1}{2} |\Phi_2^{(b)}\rangle e^{-i\lambda_2^{(b)} t} \\
+ \frac{J_1}{2\sqrt{J_1^2 + J_2^2 - J_2\sqrt{J_1^2 + J_2^2}}} |\Phi_3^{(b)}\rangle e^{-i\lambda_3^{(b)} t} - \frac{1}{2} |\Phi_4^{(b)}\rangle e^{-i\lambda_4^{(b)} t}.
$$

Note that $\lambda_1^{(b)} - \lambda_3^{(b)} = \lambda_2^{(b)}$, $\lambda_4^{(b)} - \lambda_2^{(b)} = \lambda_3^{(f)}$, and $\lambda_4^{(b)} - \lambda_4^{(b)} = \lambda_4^{(f)}$. As a result, the fidelity of state transfer, $\mathcal{F}(t) \equiv |\langle\Psi(t)|\uparrow\uparrow\uparrow\downarrow\rangle|^2$, is the same for both fermions ($\kappa \to \infty$) and bosons with $\kappa = 1$, which holds true for $N_i = 1$ and any $N$. 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 $\lambda_1^{(b)} = \sqrt{\frac{7}{2}}J_2$, $\lambda_2^{(b)} = \lambda_1^{(b)} + J_2$, $\lambda_3^{(b)} = \lambda_1^{(b)} + 2J_2$, 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 inter-species interaction is much larger than the intra-species interaction. Then the two lowest eigenstates $|\Phi_1^{(b)}\rangle \simeq \frac{1}{\sqrt{2}}(|0, 0, 0, 1\rangle + |1, 0, 0, 0\rangle)$ and $|\Phi_2^{(b)}\rangle \simeq \frac{1}{\sqrt{2}}(|1, 0, 1, 1\rangle + |0, 1, 0, 1\rangle)$ become degenerate, $\lambda_1^{(b)} \simeq \lambda_2^{(b)}$, and separated from the other two eigenstates $|\Phi_3^{(b)}\rangle \simeq \frac{1}{\sqrt{2}}(|0, 1, 1, 1\rangle + |1, 1, 0, 1\rangle)\ simeq \frac{1}{\sqrt{2}}(|0, -1, 1, 1\rangle + |1, -1, 0, 1\rangle)$ by $\lambda_3^{(b)} - \lambda_1^{(b)} \simeq 2J_2 \pm J_2$. The state transfer between the initial $|\downarrow\uparrow\uparrow\uparrow\rangle$ and final $|\uparrow\uparrow\downarrow\downarrow\rangle$ states proceeds then via non-resonant intermediate states $|\downarrow\downarrow\uparrow\uparrow\rangle$ and $|\uparrow\uparrow\downarrow\downarrow\rangle$ as a third-order process with the effective Rabi frequency $J_{\text{eff}} \simeq \frac{J_1J_2J_4}{(2J_2)^3} \simeq \frac{\kappa^2 J_2^3}{4J_2^3}$.

**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 $N_i = 1$ and assume weak magnetic field $B(x) = b(x)/g$ ($g \gg 1$) which modifies the Hamiltonian $H$ of Eq. (1) in the main text as $\tilde{H} = H + \sum_{i=1}^{N-1} \frac{b(x_{i+1}) - b(x_i)}{g}$. For the corresponding energy of $N$-particle eigenfunction $\Phi$, to linear order in $1/g$, we then obtain

$$
\tilde{E} = E - 2 \sum_{j=1}^{N} \frac{\beta_j}{g} \frac{\partial^2}{\partial \beta_j} + \sum_{j=1}^{N} \beta_j,
$$

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

$$
\beta_j = \frac{\int \prod_{i=1}^{N-1} dx_{i+1} dx_{i+1} \langle \Psi_0 | 2b(x_{i+1}) \rangle \langle \Psi_0 | x_{i+1} : x_{i+1} \rangle |^2}{\int \prod_{i=1}^{N-1} dx_{i+1} dx_{i+1} \langle \Psi_0 | x_{i+1} : x_{i+1} \rangle |^2},
$$

where in $\Psi_0$ in the numerator the spin-down particle $x_{i+1}$ is placed at position $j$. The effective spin Hamiltonian for the case $\kappa \to \infty$ can now be cast as

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

with $h_j = \beta_j$. 
