Effective three-body interactions in triangular optical lattices

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We demonstrate that a triangular optical lattice of two atomic species, bosonic or fermionic, can be employed to generate a variety of spin-1/2 Hamiltonians. These include effective three-spin interactions resulting from the possibility of atoms tunneling along two different paths. Such interactions can be employed to simulate particular one- or two-dimensional physical systems with ground states that possess a rich structure and undergo a variety of quantum phase transitions. In addition, tunneling can be activated by employing Raman transitions, thus creating an effective Hamiltonian that does not preserve the number of atoms of each species. In the presence of external electromagnetic fields, resulting in complex tunneling couplings, we obtain effective Hamiltonians that break chiral symmetry. The ground states of these Hamiltonians can be used for the physical implementation of geometrical or topological objects.

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I. INTRODUCTION

With the development of optical lattice technology [1–3], considerable attention has been focused on the experimental simulation of a variety of many-particle systems, such as spin chains [4–7]. This provides the possibility to probe and realize complex quantum models with unique properties in the laboratory. Such examples, which are of interest in various areas of physics, are the systems that include many-body interactions. The latter have been hard to study in the past due to the difficulty in controlling them externally and isolating them from the environment [8]. To overcome these problems, techniques have been developed in quantum optics [9–11] which minimize imperfections and impurities in the implementation of the desired structures, thus paving the way for the consideration of such "higher-order" phenomena of multiparticle interactions. Their applications could be of much interest to cold atom technology as well as to condensed matter physics and quantum information.

In this paper we obtain the interaction terms of bosonic or fermionic lattices of two species of atoms, denoted here by $\uparrow$ and $\downarrow$ (see [4,5,7]). These can be two different hyperfine ground states of the same atom coupled via an excited state by a Raman transition. The system is brought initially into the Mott insulator phase where the number of atoms at each site of the lattice is well defined. By restricting to the case of only one atom per site it is possible to characterize the system by pseudospin-basis states provided by internal ground states of the atom. Interactions between atoms in different sites are facilitated by virtual transitions. These are dictated by the tunneling coupling J from one site to its neighbours and by collisional couplings U that take place when two or more atoms are within the same site.

In the following we consider the case of weak tunneling couplings, $J \ll U$, assuring that we are always in the Mott insulator regime. Our aim is to construct a perturbative study of the effective interactions with respect to the small parameter J/U. Up to the third order this expansion will provide Hamiltonians that include three-spin interactions. These multiparticle interactions can be, in principle, realized with near-future technology. The main physical requirement is large collisional couplings U, which can be obtained experimentally by Feshbach resonances [15–17]. First theoretical [19] and experimental [20] advances are already promising. Hence, the time interval needed for those higher-order terms to have a significant effect can be well within the coherence times of the system.

Several applications spring out from our studies. The systematic description of the low-energy Hamiltonian provides the means for the advanced control of the three-spin interactions simulated in the lattice. Hence, different physical models can be realized, with ground states that present a rich structure such as multiple degeneracies and a variety of quantum phase transitions [12–14]. Some of these multispin interactions have been theoretically studied in the past in the context of the hard rod boson [21–24], using self-duality symmetries [25,26]. Phase transitions between the corresponding ground states have been analyzed [27,28]. Subsequently, these phases may also be viewed as possible phases of the initial system—that is, in the Mott insulator, where the behavior of its ground state can be controlled at will [29].

The paper is organized as follows. In Sec. II, we present the physical system and the conditions required to obtain three-body interactions. The effective three-spin Hamiltonians for the case of bosonic or fermionic species of atoms in a system of three sites on a lattice are given in Sec. III. In Sec. IV we study the effect Raman transitions can have on the tunneling process and generalized effective Hamiltonians are presented that do not preserve the number of atoms of each species. These are of particular interest for the construction of certain geometrical evolutions. In Sec. V complex tunnelings are considered and the generation of chiral ground states is presented. In Sec. VI our results are extended toward the construction of one-dimensional models and several applications are discussed. In Sec. VII we present an outlook and the conclusions. Finally, in the Appendixes, two alternative methods are presented for the perturbation theory that results in the three-spin interactions.

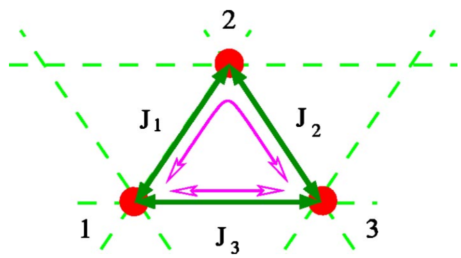

FIG. 1. (Color Online) The basic building block for the triangular lattice configuration. Three-spin interaction terms appear between sites 1, 2, and 3. For example, tunneling between 1 and 3 can happen through two different paths, directly and through site 2. The latter results in an exchange interaction between 1 and 3 that is influenced by the state of site 2.

II. PHYSICAL MODEL

Let us consider a cloud of ultracold neutral atoms superimposed with several optical lattices [4–7,30]. For sufficiently strong intensities of the laser field this system can be placed in the Mott insulator phase where the expectation value of only one particle per lattice site is energetically allowed [3]. We are interested in the particular setup of lattices that form an equilateral triangular configuration, as shown in Fig. 1. This allows for the simultaneous superposition of the positional wave functions of the atoms belonging to the three sites. As we shall see in the following this results in the generation of three-spin interactions.

The main contributions to the dynamics of the atoms in the lattice sites are given by the collisions of the atoms within the same site and the tunneling transitions of the atoms between neighboring sites. In particular, the coupling of the collisional interaction for atoms in the same site is taken to be very large in magnitude, while it is supposed to vanish when it is in different sites. Due to the low temperature of the system, this term is completely characterized by the *s*-wave scattering length. Furthermore, the overlap of the Wannier wave functions between adjacent sites determines the tunneling amplitude J of the atoms from one site to its neighbors. Here, the relative rate between the tunneling and collisional interaction terms is supposed to be very small—i.e., $J \ll U$—so that the state of the system is mainly dominated by the collisional interaction.

The Hamiltonian describing the three lattice sites with three atoms of species $\sigma=\{\uparrow,\downarrow\}$ subject to the above interactions is given by

$$H = H^{(0)} + V, \tag{2.1}$$

with

$$H^{(0)} = \frac{1}{2}\sum_{j\sigma\sigma'} U_{\sigma\sigma'} :n_{j\sigma}n_{j\sigma'}:,$$

$$V = -\sum_{j\sigma} (J_j^{\sigma} a_{j\sigma}^{\dagger} a_{j+1\sigma} + \text{H.c.}),$$

where $a_{j\sigma}$ denotes the annihilation operator of atoms of species σ at site j. The annihilation operator can describe fermions or bosons satisfying commutation or anticommutation relations, respectively, given by

$$[a_{j\sigma}, a_{j'\sigma'}^{\dagger}]_{\pm} = \delta_{jj'}\delta_{\sigma\sigma'},$$

$$[a_{j\sigma}, a_{j'\sigma'}]_{\pm} = [a_{j\sigma}^{\dagger}, a_{j'\sigma'}^{\dagger}]_{\pm} = 0, \tag{2.2}$$

where the $\pm$ sign denotes the anticommutator or the commutator. The operator $n_{j\sigma}$ is the corresponding number operator and $:\cdots:$ denotes normal ordering of the product of the creation and annihilation operators. The Hamiltonian $H^{(0)}$ is the lowest order in the expansion with respect to the tunneling interaction.

Due to the large collisional couplings activated when two or more atoms are present within the same site, the weak tunneling transitions do not change the average number of atoms per site. This is achieved by adiabatic elimination of higher-population states along the evolution leading eventually to an effective Hamiltonian (see the Appendixes). The latter allows virtual transitions between these levels, providing eventually nontrivial evolutions. As we shall see in the Appendix it is possible to describe the low-energy evolution of the bosonic or fermionic system up to the third order in the tunneling interaction by the effective Hamiltonian

$$H_{\text{eff}} = -\sum_{\gamma} \frac{V_{\alpha\gamma}V_{\gamma\beta}}{E_{\gamma}} + \sum_{\gamma\delta} \frac{V_{\alpha\gamma}V_{\gamma\delta}V_{\delta\beta}}{E_{\gamma}E_{\delta}}. \tag{2.3}$$

The indices α, β refer to states with one atom per site while γ, δ refer to states with two or more atomic populations per site, and E_{γ} are the eigenvalues of the collisional part $H^{(0)}$, while we neglected fast rotating terms effective for long-time intervals.

It is instructive to estimate the energy scales involved in such a physical system. We would like to have a significant effect of the three-spin interaction within the decoherence times of the experimental system, which we can take here to be of the order of several 10 ms. It is possible to vary the tunneling interactions from zero to some maximum value which we can take here to be of the order of $J/\hbar \sim 1$ kHz [2]. In order to have a significant effect from the term J^3/U^2 produced within the decoherence time one should choose $U/\hbar \sim 10$ kHz. This can be achieved experimentally by moving close to a Feshbach resonance [15–18], where U can take significantly large values as long as trap losses, attributed to three-body collisions or production of molecules, remain negligible. With respect to these parameters we have $(J/U)^2 \sim 10^{-2}$, which is within the Mott insulator regime, while the next order in perturbation theory is an order of magnitude smaller than the one considered here and hence negligible. Note, however, that new interaction terms arise only in fifth order in perturbation due to the triangular geometry of the optical lattice. This places the requirements of our proposal for detecting the effect of three-spin interactions within the range of possible experimental values of near-future technology.

Within the regime of single-atom occupancy per site it is possible to switch to the pseudospin basis of states of the site j given by $|\uparrow\rangle \equiv |n_{j\uparrow}=1, n_{j\downarrow}=0\rangle$ and $|\downarrow\rangle \equiv |n_{j\uparrow}=0, n_{j\downarrow}=1\rangle$. Hence, the effective Hamiltonian can be given in terms of

Pauli matrices acting on states expressed in the pseudospin basis. The symmetries of the initial Hamiltonian H restrict to a large degree the form of the low-energy expansion. For example, conservation of the atom number of each species corresponds, in the spin basis, to conservation of the total z spin. Hence, any rotation on the xy-spin plane leaves the Hamiltonian invariant. This fact limits the possible spin operators that can contribute to the effective low-energy interactions. Possible terms of the effective Hamiltonian are given by $\{\sigma_j^z\}$ for the one-body interaction, $\{\sigma_j^z\sigma_{j+1}^z, \sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y\}$ for the two-body interaction, or $\{\sigma_j^z\sigma_{j+1}^z\sigma_{j+2}^z, (\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y)\sigma_{j+2}^z\}$ for the three-body interactions where $\sigma_4 = \sigma_1$ (see Fig. 1). As we can easily verify, the three-spin operators break parity symmetry, which is explicitly given by the transformation $\uparrow \leftrightarrow \downarrow$. This indicates that their coupling coefficient should also be asymmetric with respect to this transformation, as the original atomic system possesses this symmetry. Indeed, in the next section we shall see how these terms are generated in the optical lattice setup.

Another important insight for the ground states of the presented Hamiltonians comes from the geometry of the lattice. In the case considered here, the triangular pattern allows for the generation of exotic ground states due to frustration—that is, ground states that are not minimizing the energy of the individual Hamiltonians of each link of the triangle. This effectively allows for the presence of multiple degeneracy in the ground state of the system as we shall see in particular examples.

III. EFFECTIVE THREE-SPIN INTERACTIONS

A. Bosonic model

Consider the low-energy evolution of the triangular system given in Fig. 1 of three atoms in three sites of the lattice without the application of any external field. Different rates in the tunneling parameter can then be achieved by tuning the intensities of the laser field corresponding to the different directions of the triangle. By applying the perturbative expansion (2.3) up to third order we obtain that the system can effectively be described by

$$H_{\text{eff}} = \sum_{j=1}^{3} [A_j \mathbb{I} + B_j\sigma_j^z + \lambda_j^{(1)}\sigma_j^z\sigma_{j+1}^z + \lambda_j^{(2)}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y) + \lambda^{(3)}\sigma_j^z\sigma_{j+1}^z\sigma_{j+2}^z + \lambda_j^{(4)}(\sigma_j^x\sigma_{j+1}^z\sigma_{j+2}^x + \sigma_j^y\sigma_{j+1}^z\sigma_{j+2}^y)], \quad (3.1)$$

where σ_j^α is the α Pauli matrix with the usual commutation properties $[\sigma_j^\nu, \sigma_k^\mu] = 2i\epsilon^{\nu\mu\omega}\delta_{jk}\sigma_j^\omega$. The three-spin interactions presented in the last line can be viewed as the two-spin interactions of the second line controlled by the third spin (being spin up or down) through an additional σ^z operator. The couplings, A, B, and $\lambda^{(i)}$ are given as expansions in $J^\sigma/U_{\sigma\sigma'}$ by

$$A_j = -J_1^\uparrow J_2^\uparrow J_3^\uparrow\left(\frac{3}{2U_{\uparrow\uparrow}^2} + \frac{1}{2U_{\uparrow\downarrow}^2} + \frac{1}{U_{\uparrow\downarrow}U_{\uparrow\uparrow}}\right) - J_j^{\uparrow 2}\left(\frac{1}{U_{\uparrow\uparrow}} + \frac{1}{2U_{\uparrow\downarrow}}\right) + (\uparrow \leftrightarrow \downarrow),$$

$$B_j = -\frac{J_j^{\uparrow 2} + J_{j+2}^{\uparrow}{}^2}{U_{\uparrow\uparrow}} - \frac{J_1^\uparrow J_2^\uparrow J_3^\uparrow}{U_{\uparrow\uparrow}}\left(\frac{1}{U_{\uparrow\downarrow}} + \frac{9}{2U_{\uparrow\uparrow}}\right) - (\uparrow \leftrightarrow \downarrow),$$

$$\lambda_j^{(1)} = -J_1^\uparrow J_2^\uparrow J_3^\uparrow\left(\frac{9}{2U_{\uparrow\uparrow}^2} - \frac{1}{2U_{\uparrow\downarrow}^2} - \frac{1}{U_{\uparrow\downarrow}U_{\uparrow\uparrow}}\right) - J_j^{\uparrow 2}\left(\frac{1}{U_{\uparrow\uparrow}} - \frac{1}{2U_{\uparrow\downarrow}}\right) + (\uparrow \leftrightarrow \downarrow),$$

$$\lambda_j^{(2)} = -J_j^\downarrow J_{j+1}^\uparrow J_{j+2}^\uparrow\left(\frac{3}{2U_{\uparrow\downarrow}^2} + \frac{1}{2U_{\uparrow\uparrow}^2} + \frac{1}{U_{\uparrow\downarrow}U_{\uparrow\uparrow}}\right) - \frac{J_j^\uparrow J_j^\downarrow}{2U_{\uparrow\downarrow}} + (\uparrow \leftrightarrow \downarrow),$$

$$\lambda^{(3)} = -\frac{J_1^\uparrow J_2^\uparrow J_3^\uparrow}{U_{\uparrow\uparrow}}\left(\frac{3}{2U_{\uparrow\uparrow}} - \frac{1}{U_{\uparrow\downarrow}}\right) - (\uparrow \leftrightarrow \downarrow),$$

$$\lambda_j^{(4)} = -\frac{J_j^\uparrow J_{j+1}^\uparrow J_{j+2}^\downarrow}{U_{\uparrow\uparrow}}\left(\frac{1}{2U_{\uparrow\uparrow}} + \frac{1}{U_{\uparrow\downarrow}}\right) - (\uparrow \leftrightarrow \downarrow), \quad (3.2)$$

where the symbol $(\uparrow \leftrightarrow \downarrow)$ denotes the repeating of the same term as on its left, but with the $\uparrow$ and $\downarrow$ indices interchanged. The A term contributes to an overall phase factor in the time evolution of the system and can be ignored. The B term can easily be eliminated and an arbitrary magnetic field term of the form $\Sigma_j \vec{B}\cdot\vec{\sigma}$ can be added by applying a Raman transition with the appropriate laser fields. The behavior of the effective couplings as functions of the tunneling and collisional couplings is given in Fig. 2.

One can isolate different parts of Hamiltonian (3.1), each one including a three-spin interaction term, by varying the tunneling and/or the collisional couplings appropriately so that particular terms in Eq. (3.1) vanish, while others are freely varied. An example of this can be seen in Fig. 3 where the couplings $\lambda^{(1)}$ and $\lambda^{(3)}$ are depicted. There, for the special choice of the collisional terms, $U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = 2.12U_{\uparrow\downarrow}$, the $\lambda^{(1)}$ coupling is kept to zero for a wide range of tunneling couplings, while the three-spin coupling $\lambda^{(3)}$ can take any arbitrary value. One can also suppress the exchange interactions by keeping one of the two tunneling couplings zero without affecting the freedom in obtaining arbitrary positive or negative values for $\lambda^{(3)}$ as seen in Fig. 3.

Hence, the one-dimensional Hamiltonian of the form

$$H(B_x, B_z) = -\sum_j (B_x\sigma_j^x + B_z\sigma_j^z + \sigma_j^z\sigma_{j+1}^z\sigma_{j+2}^z)$$

can be simulated in the optical lattice where all of its couplings can be arbitrarily and independently varied. The three-spin interaction term of this Hamiltonian possesses fourfold degeneracy in its ground state, spanned by the states $\{|\uparrow\uparrow\uparrow\rangle, |\uparrow\downarrow\downarrow\rangle, |\downarrow\uparrow\downarrow\rangle, |\downarrow\downarrow\uparrow\rangle\}$. The criticality behavior of this model has been extensively studied in the past [21,28], where it is shown to present first and second order phase transitions. In particular, for $B_z = 0$ its self-dual character can be demonstrated [25,26]. To explicitly show that let us define the dual operators

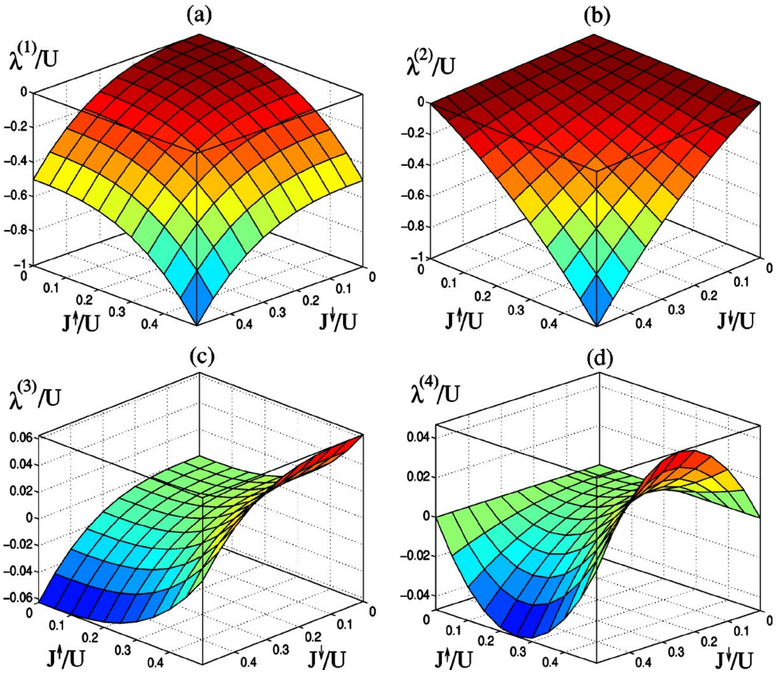

FIG. 2. (Color online) The effective couplings (a) $\lambda^{(1)}$, (b) $\lambda^{(2)}$, (c) $\lambda^{(3)}$, and (d) $\lambda^{(4)}$ as functions of the tunneling couplings $J^{\uparrow}/U$ and $J^{\downarrow}/U$, where we have set the tunneling couplings to be $J_1^{\sigma}=J_2^{\sigma}=J_3^{\sigma}$ and the collisional couplings to be $U_{\uparrow\uparrow}=U_{\uparrow\downarrow}=U_{\downarrow\downarrow}=U$. All the parameters are normalized with respect to U.

$$\overline{\sigma_j^x} \equiv \sigma_j^z\sigma_{j+1}^z\sigma_{j+2}^z, \quad \overline{\sigma_j^z} \equiv \prod_{k=0}^{\infty} \sigma_{i-3k}^x\sigma_{i-3k-1}^x,$$

which also satisfy the usual Pauli spin algebra. We can reexpress the Hamiltonian $H(B_x,0)$ with respect to the dual operators, obtaining finally

$$H(B_x,0) = B_x H(B_x^{-1},0).$$

This equation of self-duality indicates that if there is one critical point, then it should be at $|B_x|=1$ as has also been verified numerically. Furthermore, the two-spin interaction $\sigma_j^z\sigma_{j+1}^z$ has a degeneracy with a Z_2 symmetry while $\sigma_j^z\sigma_{j+1}^z\sigma_{j+2}^z$ has a threefold degeneracy leading to a Z_3 symmetry. By varying the corresponding couplings of the effective Hamiltonian it is possible to induce transitions to and from the Z_2- and Z_3-ordered phases in a similar fashion as has been theoretically demonstrated in [13].

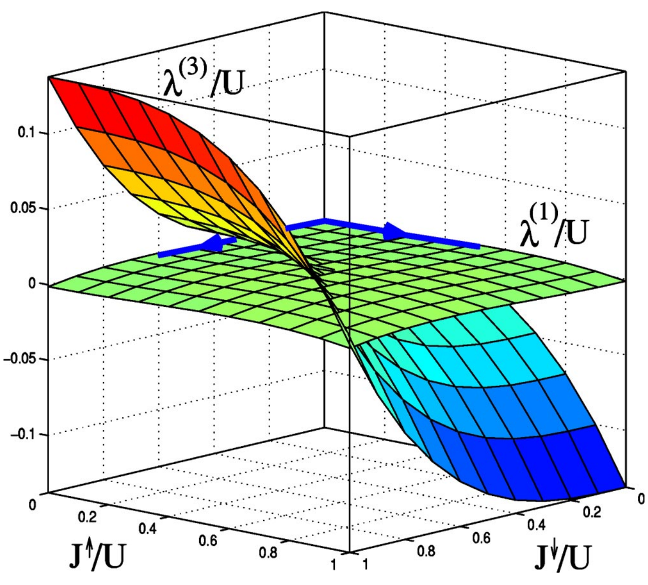

FIG. 3. (Color online) The effective couplings $\lambda^{(1)}$ and $\lambda^{(3)}$ are plotted against $J^{\uparrow}/U$ and $J^{\downarrow}/U$ for $U_{\uparrow\uparrow}=U_{\downarrow\downarrow}=2.12U$ and $U_{\uparrow\downarrow}=U$. The coupling $\lambda^{(1)}$ appears almost constant and zero as the unequal collisional terms can create a plateau area for a small range of tunneling couplings, while $\lambda^{(3)}$ can be varied freely to positive or negative values.

B. Fermionic model

Alternatively, one can consider the case of fermionic atoms and derive the effective interactions they induce up to third order. Compared to the couplings in the bosonic case we now have $U_{\uparrow\downarrow}=U$ being the only one that is present. The Pauli exclusion principle can be signaled by having $U_{\uparrow\uparrow}$, $U_{\downarrow\downarrow}\rightarrow\infty$ which eventually forbids two fermionic atoms of the same species from occupying the same site. Keeping terms up to third order in J_j^{σ}/U and employing the anticommutation relations (2.2) we obtain the effective Hamiltonian

$$H_{\text{eff}} = \sum_{j=1}^{3} [\mu_j^{(1)}(\mathbb{I} - \sigma_j^z\sigma_{j+1}^z) + \mu^{(3)}(\sigma_j^z - \sigma_1^z\sigma_2^z\sigma_3^z) + \mu_j^{(2)}(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y) + \mu_j^{(4)}(\sigma_j^x\sigma_{j+1}^z\sigma_{j+2}^x + \sigma_j^y\sigma_{j+1}^z\sigma_{j+2}^y)],$$

where the effective couplings are a function of the initial variables of the Hamiltonian (2.1) and

$$\mu_j^{(1)} = -\frac{1}{2U}(J_j^{\uparrow 2} + J_j^{\downarrow 2}), \quad \mu_j^{(2)} = \frac{1}{U}J_j^{\uparrow}J_j^{\downarrow},$$

$$\mu^{(3)} = -\frac{1}{2U^2}(J_1^{\uparrow}J_2^{\uparrow}J_3^{\uparrow} - J_1^{\downarrow}J_2^{\downarrow}J_3^{\downarrow}),$$

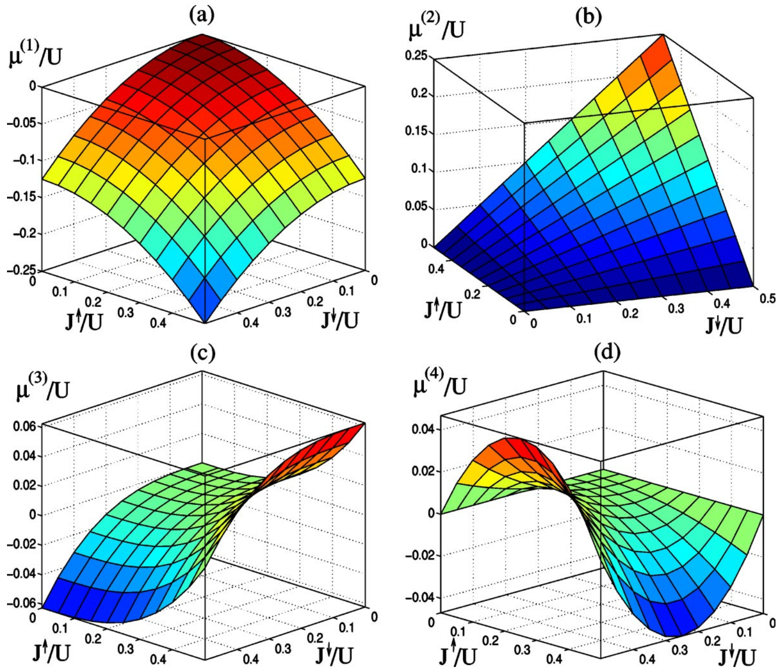

FIG. 4. (Color online) The effective couplings (a) $\mu^{(1)}$, (b) $\mu^{(2)}$, (c) $\mu^{(3)}$, and (d) $\mu^{(4)}$ as functions of the tunneling couplings $J^{\uparrow}/U$ and $J^{\downarrow}/U$, where we have set the tunneling couplings to be $J_1^{\sigma}=J_2^{\sigma}=J_3^{\sigma}$.

$$\mu_j^{(4)} = \frac{3}{2U^2}(J_j^{\uparrow}J_{j+1}^{\uparrow}J_{j+2}^{\downarrow} - J_j^{\downarrow}J_{j+1}^{\downarrow}J_{j+2}^{\uparrow}).$$

The dependence of the coupling terms on the parameters of the initial Hamiltonian is simpler than in the bosonic case. Nevertheless, they can express a similar behavior as can been seen in Fig. 4.

If the tunneling constants do not depend on the pseudospin orientation, then any three-spin interaction vanishes. Nevertheless, when the tunneling amplitudes depend on the spin and by having just one of the orientation with nonzero tunneling, then just the diagonal two- and three-spin interactions remain.

IV. RAMAN-ACTIVATED TUNNELINGS

A number of variations of the previous Hamiltonians are possible by employing techniques available from quantum optics [4,7]. An interesting example involves the application of Raman transitions during the tunneling process. These transitions involve the direct coupling of the two atomic states ↑ and ↓. Consequently they are not atom-number preserving for each of the species.

A. General case

Let us first consider the case where the atoms are strongly trapped by an optical lattice as in the previous sections. If the lasers producing the Raman transition are forming standing waves, it is possible to activate tunneling transitions of atoms that simultaneously experience a change in their internal state. As we shall see in the following the resulting Hamiltonian is given by an SU(2) rotation applied to each Pauli matrix of the Hamiltonian (3.1).

In particular, we shall consider the case of activating the tunneling with the application of two individual Raman transitions. These transitions consist of four paired laser beams L_1, L_2 and L_1', L_2', each pair having a blue detuning Δ and Δ', different for the two different transitions. The phases and amplitudes of the laser beams can be properly tuned so that the first Raman transition allows the tunneling of the state

$$|+\rangle \equiv (\cos\theta)|a\rangle + (\sin\theta)e^{-i\phi}|b\rangle,$$

with tunneling rate J_+ between two neighboring sites, while the second one activates the tunneling of the state

$$|-\rangle \equiv (\sin\theta)|a\rangle - (\cos\theta)e^{-i\phi}|b\rangle,$$

by an additional phase difference of π between the lasers L_1', L_2', with an effective tunneling rate J_-. In the above equations ϕ denotes the phase difference between the L_i laser field, while $\tan\theta = |\Omega_2/\Omega_1|$, where Ω_i are their corresponding Rabi frequencies. Hence, the effective tunneling term is given by

$$V_c = -\sum_i (J_+ c_i^{+\dagger} c_{i+1}^{+} + J_- c_i^{-\dagger} c_{i+1}^{-} + \text{H.c.}),$$

where the tunneling couplings J_+ and J_- are given by the potential barrier of the initial optical lattice superposed by the potential reduction due to the Raman transitions. In addition, the creation and annihilation operators are given as an SU (2) rotation of the initial ones—i.e.,

$$\begin{pmatrix} c_i^+ \\ c_i^- \end{pmatrix} = g(\phi,\theta)\begin{pmatrix} a_i \\ b_i \end{pmatrix},$$

with the unitary SU(2) matrix

$$g(\phi,\theta) = \begin{pmatrix} \cos\theta & e^{i\phi}\sin\theta \\ \sin\theta & -e^{i\phi}\cos\theta \end{pmatrix}.$$

Hence, the resulting tunneling Hamiltonian can be obtained from the initial one via an SU (2) rotation $V_c = gVg^{\dagger}$, where the corresponding tunneling couplings are formally identified—i.e., $J^+ = J^{\uparrow}$ and $J^- = J^{\downarrow}$. Note that the collisional

Hamiltonian is not affected by the Raman transitions, and hence it is not transformed under g rotations.

It is easy to derive the effective Hamiltonian for this transformation using the perturbative expansion. Indeed, from expressions (A3) and (A4) of the Appendix we straightforwardly obtain the second- and third-order terms of the Hamiltonian $\widetilde{H}_{\text{eff}}$ that appear after application of the Raman transition. They are given by an SU (2) rotation that acts on the Pauli matrices of the initial effective Hamiltonian. Actually this statement holds in all orders of the perturbation theory and reads, in its generality,

$$\widetilde{H}_{\text{eff}}^{(n)}(\phi,\theta) = g(\phi,\theta)H_{\text{eff}}^{(n)}g^{\dagger}(\phi,\theta),$$

where n is the order of the perturbation. Note that this useful result holds not only for the ϕ rotations, but also for the θ rotations, which, in general, do not commute with the collisional Hamiltonian $H^{(0)}$.

B. Rotated anisotropic *XY* model

We now show that the above-presented Raman transitions can be employed to obtain, for example, the anisotropic XY model. The direction of anisotropy is determined by the phase difference of the laser fields employed for the Raman transition. In particular consider, as in the previous, three sites of the optical lattice in a equilateral triangular configuration. For simplicity we assume $J_+ = J_- = J$ and $U_{\uparrow\uparrow} = U_{\downarrow\downarrow} = U_{\uparrow\downarrow} = U$. Then the effective Hamiltonian to the third order becomes the rotation

$$\widetilde{H}_{\text{eff}}(\phi,\pi/2) = g(\phi)\widetilde{H}_{\text{eff}}g^{\dagger}(\phi), \quad (4.1)$$

where $g(\phi) = g(\phi,\theta=0)$ is a z-axis rotation and $\widetilde{H}_{\text{eff}}$ is the $\theta = \pi/2$ rotated effective Hamiltonian around the y axis given by

$$\widetilde{H}_{\text{eff}} = \sum_{i=1}^{3} (A\mathbb{I} + B\sigma_i^x + \nu^{(1)}\sigma_i^x\sigma_{i+1}^x + \nu^{(3)}\sigma_i^x\sigma_{i+1}^x\sigma_{i+2}^x),$$

with

$$A = -\frac{3}{2}\frac{J^2}{U} - 3\frac{J^3}{U^2}, \quad B = -2\frac{J^2}{U} - \frac{11}{2}\frac{J^3}{U^2},$$

$$\nu^{(1)} = -\frac{1}{2}\frac{J^2}{U} - 3\frac{J^3}{U^2}, \quad \nu^{(3)} = -\frac{1}{6}\frac{J^3}{U^2}.$$

These effective couplings agree with the ones presented in Eqs. (3.2). Moreover, by controlling the amplitude of the initial standing waves that trap the atoms in their equilibrium positions it is possible to reactivate the tunnelings $J^{\uparrow}$ and $J^{\downarrow}$. This has the effect that the overall Hamiltonian is the sum of the two Hamiltonians, the rotated one (4.1) and the initial one (3.1).

One can now check that the Hamiltonian (3.1) is invariant under $g(\phi)$ rotations. On the other hand, when we add the Hamiltonians $\widetilde{H}_{\text{eff}}$ and the one from Eq. (3.1) we obtain the generalized version of the anisotropic XY model where additional third-order terms are present. Hence, by turning on the $J^{\uparrow}$ and $J^{\downarrow}$ tunnelings we can obtain the rotated version of the anisotropic XY model, where the rotation is performed with respect to the z-spin axis by an angle ϕ. This approach provides a variety of control parameters (e.g., the angle ϕ and the ratio of the couplings of the two added Hamiltonians) and, in addition, one can have these variables independent for each of the three directions of the two-dimensional optical lattice. Particular settings of these structures have been proven to generate topological phenomena [7], which support exotic anyonic excitations, useful for the construction of topological memories [31]. In addition, the possibility of varying arbitrarily the control parameters of the above Hamiltonians and, consequently, of their ground states gives us a natural setup to study such phenomena as geometrical phases in lattice systems. Examples will be presented elsewhere [32].

V. COMPLEX TUNNELING AND TOPOLOGICAL EFFECTS

Consider the case where we employ complex tunneling couplings [33] in the transitions described above. This can be performed by employing additional characteristics of the atoms like a charge e, an electric moment $\vec{\mu}_e$ or a magnetic moment $\vec{\mu}_m$, and external electromagnetic fields. As the external fields can break time reversal symmetry, new terms of the form $\{\sigma_j^x\sigma_{j+1}^y\sigma_{j+2}^z - \sigma_j^y\sigma_{j+1}^x\sigma_{j+2}^z\}$ appear in the effective Hamiltonian. In particular, the minimal coupling of the atom with the external field can be given in general by substituting its momentum by

$$\vec{p} \rightarrow \vec{p} + e\vec{A}(\vec{x}) + \vec{\mu}_m \times \vec{E}(\vec{x}) + (\vec{\mu}_e \cdot \vec{\nabla})\vec{A}(\vec{x}),$$

where $\vec{E}$ is the electric field and $\vec{A}$ is the vector potential. All of these terms satisfy the Gauss gauge if we demand that $\vec{\nabla} \cdot \vec{A} = 0$ and $\vec{E}(\vec{r}) \propto \vec{r}/r^3$; hence, they can generate a possible phase factor for the tunneling couplings.

The first term results in the well-known Aharonov-Bohm effect [34], while the second one is the origin of the Aharonov-Casher effect [35]. The first one requires that the atoms involved be charged, which is not possible to achieve in the optical lattice setup. On the other hand it is plausible to consider the electric or magnetic moments of the atoms. Nevertheless, the Aharonov-Casher effect requires that the magnetic moment of the atom move in the field of a straight homogeneously charged line, the latter being technologically difficult to implement, although recent experiments have been performed that generalize the Aharonov-Casher effect, partly overcoming the technological obstacles [36]. The third case involves the cyclic move of an electric moment through a gradient of a magnetic field finally contributing the phase

$$\phi = \int_S (\vec{\mu}_e \cdot \vec{\nabla})\vec{B} \cdot d\vec{s}$$

to the initial state, where S is the surface enclosed by the cyclic path of the electric moment. For example, if $\vec{\mu}_e$ is perpendicular to the surface S, taken to lie on the x-y plane, then a nonzero phase ϕ is produced if there is a nonvanishing gradient of the magnetic field along the z direction. Alternatively, if $\vec{\mu}_e$ is along the surface plane, then a nonzero phase is produced if the z component of the magnetic field has a nonvanishing gradient along the direction of $\vec{\mu}_e$. Hence, it is possible to generate a phase factor contribution to the tunneling couplings $J=e^{i\phi}|J|$ with

$$\phi = \int_{\vec{x}_i}^{\vec{x}_{i+1}} (\vec{\mu}_e \cdot \vec{\nabla})\vec{A} \cdot d\vec{x}.$$

Here $\vec{x}_i$ and $\vec{x}_{i+1}$ denote the positions of the lattice sites connected by the tunneling coupling J.

In order to isolate the new terms that appear in the case of complex tunneling couplings we should restrict ourselves to purely imaginary ones—i.e., $J_j^\sigma = \pm i|J_j^\sigma|$. Then the effective Hamiltonian (2.3) becomes

$$H_{\text{eff}} = \sum_i [A\mathbb{I} + B\sigma_i^z + \tau^{(1)}\sigma_i^z\sigma_{i+1}^z + \tau^{(2)}(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y) + \tau^{(3)}(\sigma_i^x\sigma_{i+1}^y - \sigma_i^y\sigma_{i+1}^x) + \tau^{(4)}\epsilon_{lmn}\sigma_i^l\sigma_{i+1}^m\sigma_{i+2}^n], \quad (5.1)$$

where ϵ_{lmn} with $\{l,m,n\}=\{x,y,z\}$ denotes the total antisymmetric tensor in three dimensions and summation over the indices l,m,n is implied. The couplings appearing in Eq. (5.1) are given in the bosonic case by

$$A = \frac{J^{\uparrow 2}}{U_{\uparrow\uparrow}} + \frac{J^{\downarrow 2}}{U_{\downarrow\downarrow}} + \frac{J^{\uparrow 2}+J^{\downarrow 2}}{2U_{\uparrow\downarrow}}, \quad B = 2\frac{J^{\uparrow 2}}{U_{\uparrow\uparrow}} - 2\frac{J^{\downarrow 2}}{U_{\downarrow\downarrow}},$$

$$\tau^{(1)} = \frac{J^{\uparrow 2}}{U_{\uparrow\uparrow}} + \frac{J^{\downarrow 2}}{U_{\downarrow\downarrow}} - \frac{J^{\uparrow 2}+J^{\downarrow 2}}{2U_{\uparrow\downarrow}}, \quad \tau^{(2)} = \frac{J^{\uparrow}J^{\downarrow}}{U_{\uparrow\downarrow}},$$

$$\tau^{(3)} = i\frac{J^{\uparrow 2}J^{\downarrow}}{U_{\uparrow\uparrow}}\left(\frac{1}{2U_{\uparrow\uparrow}} + \frac{1}{U_{\uparrow\downarrow}}\right) + (\uparrow \leftrightarrow \downarrow),$$

$$\tau^{(4)} = i\frac{J^{\uparrow 2}J^{\downarrow}}{U_{\uparrow\uparrow}}\left(\frac{1}{2U_{\uparrow\uparrow}} + \frac{1}{U_{\uparrow\downarrow}}\right) - (\uparrow \leftrightarrow \downarrow)$$

and in the fermionic case by

$$A = -\tau^{(1)} = \frac{J^{\uparrow 2}+J^{\downarrow 2}}{2U}, \quad B = \tau^{(3)} = 0,$$

$$\tau^{(2)} = -\frac{J^{\uparrow}J^{\downarrow}}{U}, \quad \tau^{(4)} = i\frac{J^{\uparrow 2}J^{\downarrow} - J^{\downarrow 2}J^{\uparrow}}{2U^2}.$$

By taking $U_{\uparrow\downarrow}\to\infty$, $U_{\uparrow\uparrow}=-U_{\downarrow\downarrow}=-U$, $J^{\uparrow}=-J$, and $J^{\downarrow}=J$, one can set, in the bosonic case, with the aid of Feshbach resonances and compensating Zeeman terms, all the couplings to be zero apart from $\tau^{(4)}$. Hence, the effective Hamiltonian reduces to

$$H_{\text{eff}} = \tau^{(4)}\sum_{\langle ijk\rangle} \vec{\sigma}_i \cdot \vec{\sigma}_j \times \vec{\sigma}_k, \quad (5.2)$$

with $\vec{\sigma}=(\sigma^x,\sigma^y,\sigma^z)$ and $\tau^{(4)}=|J|^3/U^2$. Remarkably, with this physical proposal, the interaction term (5.2) can be isolated, especially from the Zeeman terms that are predominant in equivalent solid-state implementations. This interaction term is also known in the literature as the *chirality operator* [37].

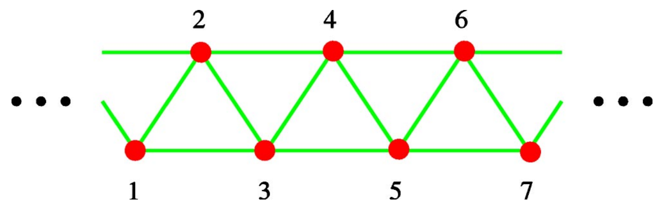

FIG. 5. (Color online) The one-dimensional chain constructed out of equilateral triangles. Each triangle experiences the three-spin interactions presented in the previous.

It breaks time reversal symmetry of the system, a consequence of the externally applied field, by effectively splitting the degeneracy of the ground state into two orthogonal sectors—namely, "+" and "−," related by time reversal T. These sectors are uniquely described by the eigenstates of H_{eff} at the sites of one triangle. The lowest-energy sector with eigenenergy $E_+=-2\sqrt{3}\tau^{(4)}$ is given by

$$|\Psi_{1/2}^+\rangle = \frac{1}{\sqrt{3}}(|\uparrow\uparrow\downarrow\rangle + \omega|\uparrow\downarrow\uparrow\rangle + \omega^2|\downarrow\uparrow\uparrow\rangle),$$

$$|\Psi_{-1/2}^+\rangle = -\frac{1}{\sqrt{3}}(|\downarrow\downarrow\uparrow\rangle + \omega|\downarrow\uparrow\downarrow\rangle + \omega^2|\uparrow\downarrow\downarrow\rangle). \quad (5.3)$$

The excited sector $|\Psi_{\pm 1/2}^-\rangle$ represents counterpropagation with eigenvalue $E_-=2\sqrt{3}\tau^{(4)}$ and it is obtained from Eqs. (5.3) by complex conjugation [37–39]. We would like to point out that, to the best of our knowledge, this is the first physical proposal where this interaction term can be isolated, especially from the Zeeman terms that are predominant in equivalent solid-state implementations. Alternative models employing cold atom technology for the generation of topologically nontrivial ground states are given in [7,40].

VI. ONE- AND TWO-DIMENSIONAL MODELS

It is also possible to employ the three-spin interactions that we studied extensively in the previous sections for the construction of extended one- and two-dimensional systems. The two-dimensional generalization is rather straightforward as the triangular system we considered is already defined on the plane. Hence, all the interactions considered so far can be generalized for the case of a two-dimensional lattice where the summation runs through all the lattice sites with each site having six neighbors.

The construction of the one-dimensional model is more involving. In particular, we now consider a whole chain of triangles in a zigzag one-dimensional pattern as shown in Fig. 5. In principle this configuration can extend our model from the triangle to a chain. Nevertheless, a careful consideration of the two-spin interactions shows that terms of the form $\sigma_i^z\sigma_{i+2}^z$ appear in the effective Hamiltonian, due to the triangular setting (see Fig. 5). Such Hamiltonian terms involving nearest- and next-to-nearest-neighbor interactions are of interest in their own right [12,13] but will not be addressed here. It is also possible to introduce a longitudinal optical lattice with half of the initial wavelength and an appropriate amplitude such that it cancels exactly those interactions, generating, finally, chains with only neighboring couplings.

In a similar fashion it is possible to avoid generation of terms of the form $\sigma_i^x\sigma_{i+2}^x+\sigma_i^y\sigma_{i+2}^y$ by deactivating the longitudinal tunneling coupling in one of the modes—e.g., the $\uparrow$ mode—which deactivates the corresponding exchange interaction.

As we are particularly interested in three-spin interactions we would like to isolate the chain term $\Sigma_i(\sigma_i^x\sigma_{i+1}^z\sigma_{i+2}^x+\sigma_i^y\sigma_{i+1}^z\sigma_{i+2}^y)$ from the $\lambda^{(4)}$ term of Hamiltonian (3.1). This term includes, in addition, all possible triangular permutations. To achieve that we could deactivate the nonlongitudinal tunneling for one of the two modes—e.g., the one that traps the $\uparrow$ atoms. The interaction $\sigma_i^z\sigma_{i+1}^z\sigma_{i+2}^z$ is homogeneous: hence, it does not pose such a problem when it is extended to the one-dimensional ladder. With the above procedures we can finally obtain a chain Hamiltonian as in Eq. (3.1) where the summation runs up to the total number N of sites.

VII. CONCLUSIONS

In this paper we presented a variety of different spin interactions that can be generated by a system of ultracold atoms superposed by optical lattices and initiated in the Mott insulator phase. In particular, we have been interested in the simulation and study of various three-spin interactions conveniently obtained in a lattice with equilateral triangular structure. They appear by a perturbation expansion to third order with respect to the tunneling transitions of the atoms when the dominant interaction is the collisions of atoms within the same site. Among the models presented here we specifically considered the $\sigma_i^z\sigma_{i+1}^z\sigma_{i+2}^z$ interaction, a third-order generalization of the rotated inhomogeneous XY model, as well as interactions that explicitly break chiral symmetry. These models can exhibit degeneracy in their ground states and undergo a variety of quantum phase transitions that can also be viewed as phases of the initial Mott insulator.

It is possible to employ quantum simulation techniques [41], in a similar fashion as for two-spin Hamiltonians, to generate effective three-spin interactions that are not possible to obtain straightforwardly from the optical lattice system. Hence, a variety of additional Hamiltonians can be obtained by considering manipulations of the above three-spin interactions with the application of appropriate instantaneous one- or two-spin transformations. The possibility to externally control most of the parameters of the effective Hamiltonians at will reenters our model as a unique laboratory to study the relationship among exotic systems such as chiral spin systems, fractional quantum Hall systems, or systems that exhibit high-T_c superconductivity [29,37]. In addition, suitable applications have been presented within the realm of quantum computation [30] where three-qubit gates can be straightforwardly generated from three-spin interactions. Furthermore, the unique properties related to the criticality behavior of the chain with three-spin interactions have been analyzed in [14] where the two-point correlations, used traditionally to describe the criticality of a chain, seem to fail to identify long quantum correlations, suitably expressed by particular entanglement measures [42].

In conclusion, we have presented a physical model that can efficiently simulate a variety of three-spin interactions. The employed optical lattice techniques give the possibility to externally manipulate and control the couplings of the interactions. The effect of these terms will eventually be significant with the improvement of experimental techniques. Importantly, the three-spin interactions can be isolated from two-spin ones or from possible Zeeman terms that are always present in the corresponding spin systems. This makes the further study of their properties an important task for future work.

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APPENDIX A: PERTURBATION THEORY

Consider the case of two species of atoms trapped in optical potentials forming a triangular configuration subject to the Hamiltonian given by Eq. (2.1). For simplicity define the diagonal free Hamiltonian to be given by $H_{ij}^{(0)}=E_i\delta_{ij}$, where E_i is either zero or proportional to U_{aa}, U_{bb}, or U_{ab}. As we have already mentioned we consider the case where tunneling couplings are much smaller than the collisional ones $J \ll U$. Then the evolution of the system is dominated by the term $H^{(0)}$. In fact, when we start from a configuration of one atom per lattice site, denoted by the subspace M of configurations, and activate small tunneling couplings, the change of atom number per site would be energetically unfavorable and is hence adiabatically eliminated.

To see this analytically we employ the interaction picture with respect to the Hamiltonian $H^{(0)}$, obtaining

$$H_{I_{ij}}(t) = V_{ij}\exp[\mathrm{i}(E_i - E_j)t/\hbar]. \tag{A1}$$

The evolution operator in the interaction picture is given by the time-ordered formula

$$\begin{aligned}\mathcal{U}_I(t,0) \equiv \mathrm{T}\exp\left[-\frac{\mathrm{i}}{\hbar}\int_0^t H_I(t')dt'\right] &= \mathbb{I} - \frac{\mathrm{i}}{\hbar}\int_0^t H_I(t')dt' \\ &- \frac{1}{\hbar^2}\int_0^t dt'\int_0^{t'} dt'' H_I(t')H_I(t'') \\ &+ \frac{\mathrm{i}}{\hbar^3}\int_0^t dt'\int_0^{t'} dt''\int_0^{t''} dt''' H_I(t')H_I(t'')H_I(t''') \\ &+ O((Jt)^4).\end{aligned} \tag{A2}$$

Higher orders are negligible as long as times t are considered for which Jt remains sufficiently small, while Ut is large enough to avoid the accumulation of population outside the subspace M. The latter condition is necessary to exempt fast-rotating phase factors appearing when performing the above time integrals. These phase factors are of the form $e^{i\omega t}-1$ and

$$\lim_{t\to\infty}(e^{i\omega t}-1)=\lim_{t\to\infty}\left(-2\sin^2\frac{\omega t}{2}+i\sin\omega t\right)$$
$$=(-\omega^2 t\pi+i2\pi\omega)\delta(\omega),$$

which is zero for $\omega\propto E_i-E_j\neq 0$. These conditions are in agreement with the previous demands that Jt be very small while Ut be relatively large. Hence, we can directly calculate each term of the expansion (A2) without having to take into account fast-rotating terms.

The effective Hamiltonian H_{eff} that corresponds to this evolution can be obtained by a term proportional to time t in the expansion of the evolution operator—i.e.,

$$\mathcal{U}_I(t,0)=\mathbb{I}-\frac{\mathrm{i}}{\hbar}H_{\text{eff}}t+O(t^2).$$

Consider now the second term on the right-hand side of Eq. (A2). This term gives no evolution within the subspace M of states as the tunneling Hamiltonian term V moves these states necessarily out of the M configurations. The third term gives (see [[5]])

$$(H_{\text{eff}}^{(2)})_{\alpha\beta}=-\sum_{\gamma}\frac{V_{\alpha\gamma}V_{\gamma\beta}}{E_\gamma},\qquad\text{(A3)}$$

where α and β indicate states in M, γ indicates states out of M, and E are the eigenstates of $H^{(0)}$, where we have used $E_\alpha=E_\beta=0$. This gives the usual second-order effective Hamiltonian presented in detail in [5,7]. Consider now three sites and the effect of the third term in Eq. (A2). Finally, we obtain the effective Hamiltonian with matrix elements:

$$(H_{\text{eff}}^{(3)})_{\alpha\beta}=\sum_{\gamma\delta}\frac{V_{\alpha\gamma}V_{\gamma\delta}V_{\delta\beta}}{E_\gamma E_\delta}.\qquad\text{(A4)}$$

With formulas (A3) and (A4) one can perform the perturbation up to third order and find the desired three-spin interactions (2.3). In practice the evaluation of the terms that contribute to the three-spin Hamiltonian is quite simple. The states corresponding to γ and δ include sites with two or three atoms of the same or of different species. Hence, $E_\gamma,E_\delta\propto U_{\sigma\sigma'}$. Next you need to consider the different evolutions of the form $\alpha\to\gamma\to\delta\to\beta$ that populations undertake. The tunneling couplings J^σ are determined by each of these transitions, and an appropriate coefficient is obtained in the case of the bosonic generation or annihilation of two atoms of the same species in one site.

APPENDIX B: ADIABATIC ELIMINATION

As an alternative procedure it is possible to eliminate the fast oscillating term without performing the perturbative expansion. This elimination is related to the adiabatic elimination of the states with two or more atoms per lattice site that are separated from the states with one atom per lattice site (configurations in M) by a large energy gap proportional to $U_{\sigma\sigma'}$. In fact, if we set a decomposition of the three site in terms of basis states of the form $|i_1j_1;i_2,j_2;i_3,j_3\rangle$ where 1, 2, 3 denote the site and i_k and j_k denote the number of atoms of species $\uparrow$ and $\downarrow$, respectively, in site k, we can write the general state of the three sites as

$$|\Psi(t)\rangle=\sum_{i_k,j_k}c^{i_1i_2i_3}_{j_1j_2j_3}(t)|i_1j_1;i_2,j_2;i_3,j_3\rangle.$$

By employing the Schrödinger equation we can obtain time-differential equations of the coefficients $c^{i_k}_{j_k}$ of the form

$$i\hbar\dot{c}^{i_k}_{j_k}=\sum_{i_k',j_k'}H^{i_kj_k}_{i_k'j_k'}c^{i_k'}_{j_k'},\qquad\text{(B1)}$$

where $H^{i_kj_k}_{i_k'j_k'}=\langle c^{i_k}_{j_k}|H|c^{i_k'}_{j_k'}\rangle$. It is easy to verify that the elements of H with indexes (i_kj_k) corresponding to states that do not belong to M include fast rotating phases and, hence, they are zero—i.e., for those states $\dot{c}^{i_k}_{j_k}=0$. This provides a set of linear equations of the form $\sum_{i_k',j_k'}H^{i_kj_k}_{i_k'j_k'}c^{i_k'}_{j_k'}=0$, which can be solved, in principle, explicitly. In our case, Eq. (B1) has overall 56 equations resulting from the Schrödinger equation with 48 reduced to a linear system of coupled algebraic equations. This set can be solved by a computer and then expanded in terms of small couplings $J\ll U$, obtaining an alternative verification of the previous perturbative expansion.

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