Implementation of Spin Hamiltonians in Optical Lattices

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We propose an optical lattice setup to investigate spin chains and ladders. Electric and magnetic fields allow us to vary at will the coupling constants, producing a variety of quantum phases including the Haldane phase, critical phases, quantum dimers, etc. Numerical simulations are presented showing how ground states can be prepared adiabatically. We also propose ways to measure a number of observables, like energy gap, staggered magnetization, end-chain spins effects, spin correlations, and the string-order parameter.

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In condensed matter physics, there are strongly correlated systems of spins and electrons whose study is extremely difficult both analytically and numerically. These systems are of great practical interest since they may be relevant in some important instances like high-T_c superconductivity, to quote just one open problem of great relevance. These open problems have triggered a great number of models formulated by means of quantum-many-body Hamiltonians like Heisenberg, *t*-*J*, Hubbard, etc. Their quantum phase diagrams remain unknown for generic values of coupling constants, electron concentration (doping), and temperature, although great insight is provided by particular 1D integrable models.

Quantum spin chains and ladders are one of the simplest but most emblematic quantum-many-body systems. Here we will show how to implement them using cold atoms in optical lattices. For concreteness, we will focus on spin chains first. According to Haldane's seminal work [1], the 1D integer-spin Heisenberg antiferromagnets have a unique disordered ground state with unbroken rotational symmetry and with a finite excitation gap in the spectrum, while half-integer antiferromagnets are gapless and critical. These quantum-many-body phenomena are different from the usual source of gaps in magnets; namely, single-ion anisotropy, which does not involve quantum correlation effects. Nowadays, several theoretical developments [1,2] and strong numerical evidences support Haldane's claim.

For integer spin, $s = 1$, there is a Hamiltonian that exhibits a rich phase structure, including all relevant information pertaining to the Haldane phase. This is the quadratic-biquadratic (QB) Hamiltonian

$$H_{\rm QB} = \alpha \sum_{i=1}^{N-1} [\vec{S}_i \cdot \vec{S}_{i+1} - \beta(\vec{S}_i \cdot \vec{S}_{i+1})^2] + \sum_{i=1}^{N} \vec{B}_i \vec{S}_i. \quad (1)$$

Here, $\vec{S}_i$ is the spin on the ith site, β is a relative coupling constant, and the sign of α determines the ferro or antiferromagnetic (AF) regimes. The properties of the ground state without magnetic field, $\vec{B} = 0$, are entirely determined by an angle, θ, such that $\alpha = |a| \cos(\theta)$ and $\alpha\beta = -|a| \sin(\theta)$ [see Fig. 1(a)]. For $\theta \in [-\frac{\pi}{4}, \frac{\pi}{4}]$, the ground state belongs to the Haldane phase, with $\theta = 0$ being the Heisenberg point and $\theta = \arctan(\frac{1}{3})$ the Affleck-Kennedy-Lieb-Tasaki (AKLT) point [2], which is of particular importance because it can be described with an exact valence-bond wave function. There are two critical points on which the standard correlation length diverges. At the Uimin-Lai-Sutherland (ULS) critical point [3], $\theta = \frac{\pi}{4}$, a phase transition occurs into a gapless phase. The Takhtajan-Babujian (TB) critical point [4], $\theta = -\frac{\pi}{4}$, displays a second order phase transition into a dimerized phase thus gapped, and with an exactly solvable model at $\theta = -\frac{\pi}{2}$ [5]. It has been conjectured that a quantum nondimerized nematic phase also exists [6] in the ferromagnetic region.

Likewise, ladders of spin $s = \frac{1}{2}$ [7] exhibit a rich quantum phase structure depending on their number of legs and couplings: while for odd legs they are gapless, even-legged ladders are gapped and can be in Haldane and dimerized phases, like the integer-spin one-dimensional chains. Theoretically, spin ladders are regarded as a route to approach the more complicated physics of two-dimensional quantum spin systems as we increase the number of legs. For instance, a two-leg ladder is gapped and upon hole doping serves as a toy model for studying superconducting correlations.

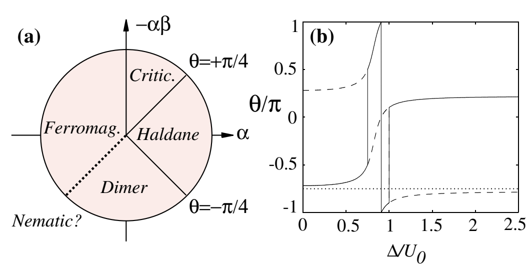

FIG. 1 (color online). (a) Different phases of the ground state of Eq. (1). (b) Type of Hamiltonian (3) as a function of the gradient of the electric field, Δ, for $U_0 = 0.75U_2$. The solid line is obtained naturally, the dashed line when working with the upper part of the spectrum. The conjectured nematic phase (dotted line) is achieved for $U_0 = U_2$ or $\Delta \to \infty$.

Experimental attempts to implement the QB Hamiltonian in real materials date back to the 1960s. The first experimental evidence of a biquadratic term was found in Mn-doped MgO [8] and for $S = 5/2$ Mn^{++} ions in antiferromagnetic chains of MnO [8]. The measured coupling constant was $\beta = -0.05$, too small and with a fixed sign. Thus, only the pure Heisenberg AF model and its immediate surroundings with a very small β are of feasible practical implementation. Experimentally, ladders are realized by selective stoichiometric composition of cuprate planes in superconductors [9]. However, residual nonvanishing interladder couplings on the planes introduce disturbances which are difficult to control.

Finding an experimental setup for checking the validity and observing the several phases of the QB Hamiltonian and of spin ladders is considered a very important challenge in the field. In this Letter we propose to solve this problem using cold atoms confined in an optical lattice [10]. As shown before, a Mott phase [11] of cold atoms in a lattice can be described using ferromagnetic spin $s = \frac{1}{2}$ [12,13] or $s = 1$ [14,15] Hamiltonians. Here we describe how to access a wider family of models, including Haldane phases of antiferromagnetic $s = 1$ chains and $s = \frac{1}{2}$ ladders. We also design a technique to prepare adiabatically the atoms in the ground state, an important task since these spins cannot be cooled. Finally we study how to detect the different spin phases and to directly observe correlation and excitation properties.

Let us first describe how to engineer Hamiltonian (1) using spin $s = 1$ bosons in an array of 1D optical lattices. For a strong confinement and low densities, the effective Hamiltonian is the Bose-Hubbard model [11]

$$H = -J \sum_{\langle j,l\rangle,\alpha} (a^\dagger_{j\alpha} a_{l\alpha} + a^\dagger_{l\alpha} a_{j\alpha}) + \sum_{j,\alpha} (E_j + B_{j\alpha}) a^\dagger_{j\alpha} a_{j\alpha} + \sum_{S=0,2} \frac{U_S}{2} \sum_{j,\alpha,\beta,\gamma,\delta} (\Psi^{(S)}_{\sigma,\gamma\delta} a_{j\gamma} a_{j\delta})^\dagger (\Psi^{(S)}_{\sigma,\alpha\beta} a_{j\alpha} a_{j\beta}). \tag{2}$$

First of all, while the indices j and l run over the lattice sites, the Greek letters label the projection along the Z axis of either the spin of an atom ($\alpha, \beta, \gamma, \delta = -1, 0, +1$) or of a pair of them ($\sigma = -2, -1, 0, 1, 2$). Then the first term in the Hamiltonian models the single-particle hopping and J is the tunneling amplitude to a neighboring site. The second term is the on site interaction between bosons. Because of symmetry, two bosons can occupy the same site only if their total spin is $S = 0$ or 2, and the interaction may itself depend on the total spin. This is taken into account by the interaction strengths, U_S, and the tensors $\Psi^{(S)}_{\sigma,\gamma\delta} = \langle S, \sigma | s, \gamma; s, \beta\rangle$, which are the Clebsch-Gordan coefficients between states $|s = 1, \gamma\rangle \otimes |s, \beta\rangle$ and $|S = 0, 2; \sigma\rangle$. Finally, we have included effective electric and magnetic fields, E_j and $B_{j\alpha}$, that can be engineered using Stark shifts and spatially dependent magnetic fields, as in current experiments [10].

We will assume that the lattice has been loaded with one atom per site [16] and that the tunneling has been strongly suppressed, $J \ll U_S$. With a perturbative calculation around states with unit occupation [13–15] we obtain the QB Hamiltonian (1) with constants

$$\alpha = \frac{1}{2} C_2, \qquad \alpha\beta = -\frac{1}{6}(2C_0 + C_2), \qquad C_S = \frac{J^2 U_S}{\Delta^2 - U_S^2}. \tag{3}$$

This result is valid only if the gradient of the magnetic field is small, $|B_{j+1} - B_j| \ll |U_S|$, and the gradient of the electric field is constant, $\Delta = E_{j+1} - E_j$, and not resonant with the interaction, $|nU_S \pm \Delta| \gg J, \forall n \in \mathbb{Z}$.

In the absence of electric or magnetic fields, the model reduces to that of [14,15], and we are restricted to a fixed value of θ, typically in the ferromagnetic sector. However, with our tools, it is possible to explore many other phases and achieve almost all values of θ (Fig. 3). The idea is to change the gradient of the electric field and use a duality $H_{AF} = -H_F$ between ferro and antiferromagnetic models. The highest energy state of a ferromagnetic model ($\alpha < 0$) is the same and exhibits the same dynamics as the ground state of the dual model ($-\alpha, -\beta$), since $(i\partial_t - H_F)\psi(t) = 0 \Leftrightarrow (i\partial_t - H_{AF})\psi^\star(t) = 0$. This equivalence is possible in current experiments because dissipation is negligible and decoherence affects equally both ends of the spectrum.

A similar procedure is used for implementing ladders [7] of spin $s = \frac{1}{2}$. A ladder is nothing but the combination of two spin chains (legs) that interact with each other. To build them we need to set up a 3D lattice that confines the atoms on planar square lattices (hopping has been suppressed along the Z direction), and superimpose along the Y direction a second 1D lattice with twice the period [Fig. 2(b)]. Adjusting the intensities of different lattices we can modify the tunneling along the leg of a ladder and between neighboring legs and completely suppress tunneling between ladders. With the help of electric and magnetic fields [13], and the duality between ferro and antiferromagnetic models, we achieve once more a full tunability of the Hamiltonian.

Let us now study how to prepare ground states adiabatically. We will focus on the Haldane phase of the $s = 1$ lattice and on the antiferromagnetic $s = \frac{1}{2}$ ladders. Since in both cases we seek an antiferromagnetic state, we can begin with a configuration of antiparallel spins, an effective staggered magnetic field, $B_j = (-1)^j |B(t)|$, and no hopping. We then progressively decrease the magnetic field and increase the interaction, α [See Fig. 3(a)]. This procedure constrains us to a subspace of fixed magnetization, $\langle \sum_j S^z_j \rangle \simeq 0$, and also ensures that the minimum energy gap between the ground state and the first excitations remains independent of the number of spins. Thus, the speed of the adiabatic process can be the same for all lattice sizes, an important point in a setup with defects.

We have studied numerically the fidelity of the adiabatic process for the AKLT point, for $\beta = 0$, and for a $s = \frac{1}{2}$

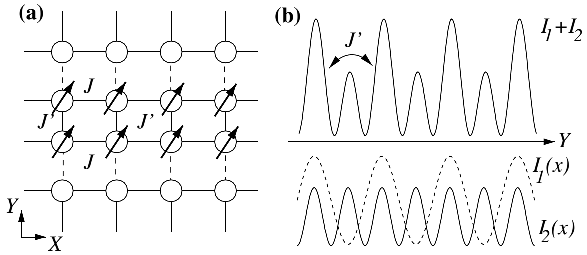

FIG. 2. (a) A ladder is the combination of two spin chains that interact with each other. Interactions along a chain and between legs can be different. (b) We can build a ladder combining a 3D lattice, $I_2(x)$, with an additional 1D optical lattice, $I_1(x)$, that has twice the period of the first one. This induces a tunable hopping J', different from the longitudinal one, J, and suppresses hopping between neighboring ladders.

ladder, using different speeds and sizes. The fidelity is the projection of the final state onto the (degenerate) ground states (in the case of $s = 1$, it is one singlet and three triplet states). The results are shown in Fig. 3(b). Already for a duration of $10h/[\max\alpha(t)]$ the Haldane phase is built with 99% fidelity. Assuming current optical lattices, with $U/h \simeq 3$ KHz and $J = 0.3U$, this implies a time of roughly 37 ms. Improvements on these values are expected with the implementation of optically induced Feschbach resonances [17].

Regarding the staggered magnetic field, for ^{87}Rb in the $F = 1$ hyperfine state, it can be produced with a weaker optical lattice, aligned with the atomic chains and made of a pair of counterpropagating laser beams in a lin $\perp$ lin configuration. If the lasers are far off resonance from the transition $^2S \rightarrow {}^2P$, we will obtain a state-dependent potential $V_\perp(x) \propto 2 + [\sin(kx)^2 - \cos(kx)^2]S_z$, where the $\sin(kx)$ and $\cos(kx)$ come from the Stark shifts induced by the σ_+ and σ_- polarizations on the atomic states. Choosing the orientation of the counterpropagating beams so that $V_\perp(x)$ has twice the periodicity of the confining lattice we get our staggered magnetic field. A similar setup can be designed for $s = \frac{1}{2}$ particles.

Once we have constructed the ground state, we would like to study its properties. We will describe a number of possible experiments, sorted by increasing difficulty. For illustrative purposes, we consider the Haldane phase of a $s = 1$ spin chain, but we want to emphasize that the same techniques can be applied to other phases, spin models, and even ladders. Preliminary evidences of the Haldane phase are obtained by studying global properties, such as the staggered magnetization, $\vec{S}_{st} = \sum_j (-1)^j \vec{S}_j$, which is zero in the dimer phase and nonzero in the Haldane phase. To measure $S_{\rm st}^{x,y}$, we apply a $\pi/2$ rotation around the Z axis using the staggered magnetic field, and then measure $\langle \sum_i S_i^{x,y} \rangle$. The remaining component $S_{\rm st}^z$ can be obtained by rotating all spins an angle $\pi/2$ around the X or Y axes, and then measuring $S_{\rm st}^y$ or $S_{\rm st}^x$.

We can also study the energy gap between the ground state and its excitations using an oscillating magnetic field, $B_j(t) = (-1)^j B \sin(\omega t)$. From linear response theory we know that for small intensities, $|B| \ll \alpha$, there is a strong resonance at the gap, $\hbar\omega = E_{\rm gap}$, which manifests itself on the growth of the staggered magnetization, $S_{\rm st}^z$. This result has been confirmed by numerical simulations of small lattices, as shown in Fig. 4.

Another interesting feature of the Haldane phase is its fractionalization effect. To understand this, one should visualize each atom with spin $s = 1$ as being composed of two $s = \frac{1}{2}$ bosons in a symmetric state. The ground state of Eq. (1) can then be built—either approximately, if $\beta \neq 1/3$, or exactly, for the AKLT—by antisymmetrizing pairs of virtual spins from neighboring sites [2]. This leaves us with two free effective $s = \frac{1}{2}$ spins at the ends of a chain, which manifest themselves physically. First, the four almost degenerate ground states are determined by the values of the free virtual spins, which we will denote as $|i_1, i_{2N}\rangle$. Thus, if the state of the system is $|\psi\rangle = \sum_{ij} c_{ij} |i, j\rangle$, the probability of measuring the left- and rightmost real spins in states $I, J = \pm 1$ is approximately $4|c_{I/2,J/2}|^2/9$. Second, the virtual spins almost do not interact and can be manipulated independently with weak magnetic fields that have different values on the borders of a chain. For instance, if we prepare the ground state using our method, apply a global rotation of angle $\theta = \frac{\pi}{2}$ around the Y axis, and then switch on the staggered magnetic field, we will measure

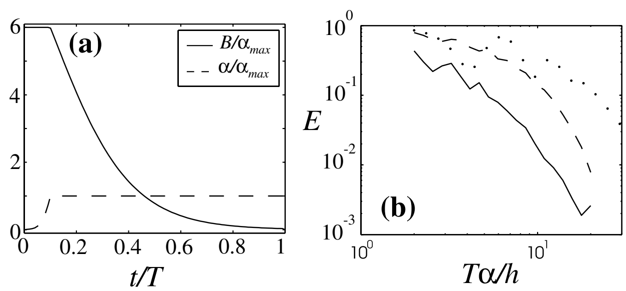

FIG. 3. (a) Procedure for the adiabatic construction of the ground state of the $s = 1$ AF with open boundary conditions. (b) Infidelity of the final state for the AKLT (dashed line), Heisenberg (solid line), and $s = \frac{1}{2}$ spin ladder (dotted line), versus duration of the process, for either nine spins (chains) or rungs (ladders).

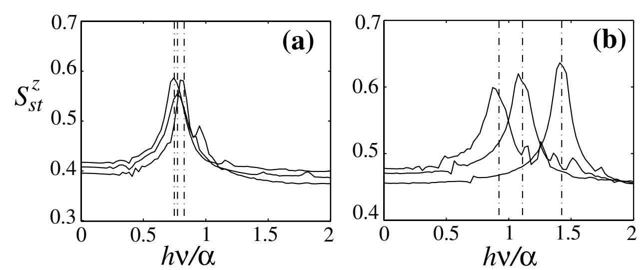

FIG. 4. Maximum staggered magnetization per spin acquired by the ground state of the (a) AKLT and (b) Heisenberg models, under an oscillating magnetic field, $B_j = (-1)^j 0.025\alpha \times \cos(2\pi\nu t)$, for five, seven, and nine spins (right to left). Vertical lines mark the finite excitation gap for the given size.

periodic oscillations in the value of $S^x_{\rm st}$, because the virtual spins on even and odd sites rotate with opposite senses.

We also have developed a procedure to measure spin correlation functions in optical lattices, an essential tool for experiments with spin lattices. Our proposal only assumes that we can trap atoms in separate lattices and empty lattice sites with double occupation [18]. First of all, we notice that a spin correlation may be written as a density correlation, $\langle S^z_j S^z_k\rangle = \langle n^{+1}_j n^{+1}_k + n^{-1}_j n^{-1}_k - n^{+1}_j n^{-1}_k - n^{-1}_j n^{+1}_k\rangle$, where n^α_k is the number of atoms in hyperfine state α on the kth site. A correlation such as $\sum_j\langle n^1_j n^1_{j+\Delta}\rangle$ can be measured by moving the atoms of species $+1$ just Δ sites [19,20], emptying all doubly occupied sites and counting the number of atoms left in state $+1$, on the sites j and k. If we rather count the atoms in state 0, then we will obtain $\langle n^{-1}_j n^{+1}_k\rangle$. With this method, and some global rotation of the spins, it is possible to obtain all correlators, $\langle \vec{S}_j \vec{S}_{j+\Delta}\rangle$. If we cannot address individual atoms, using the same procedure and measuring total populations, $\sum_k n^\alpha_k$, we will obtain averaged values, $\sum_k\langle \vec{S}_j \vec{S}_{j+\Delta}\rangle$. Both quantities are interesting to discriminate between the different spin phases.

On a much higher level of difficulty, but with pretty much the same tools as for measuring correlations we can obtain the *string-order parameters* [21]. One can show that it is equivalent to a correlation function measured on a transformed state,

$$S_{km} := \langle S^z_k e^{i\pi \sum_{j=k+1}^{m-1} S^z_j} S^z_m\rangle_\psi = \langle S^z_k S^z_m\rangle_{U_{m-k}\psi}, \qquad (4a)$$

$$U_\Delta = \exp\left[i\pi \sum_{k=1}^{N} \sum_{j=k+1}^{k+\Delta} (1 - S^{z2}_k) S^x_j \right]. \qquad (4b)$$

The unitary operation U_Δ can be performed as follows. First we perform half a swap between the $+1$ and -1 states, $U_1 = \exp[i\pi/2 \sum_k (|+1\rangle\langle -1|_k + |-1\rangle\langle +1|_k)]$, with a $\pi/2$ Raman pulse that connects these states. Next we split the three species into three optical lattices. The atoms in state 0 will move $\Delta - 1$ sites to the right, and on each movement a controlled collision with atoms in state $+1$ will take place. Adjusting the duration of this collision so that it produces a phase of π, we obtain the transformation $U_2 = \exp[i\sum_k \sum_{j=1}^{\Delta-1} \pi(|0\rangle\langle 0|_k |+1\rangle\langle +1|_{k+j})]$. We restore all atoms back to their positions and repeat the operation U_1, concluding the total transformation $U_\Delta = U_1 U_2 U_1$. Finally, we perform all required steps to measure either $\langle S^z_k S^z_{k+\Delta}\rangle$ or $\sum_k\langle S^z_k S^z_{k+\Delta}\rangle$.

Typical experiments have defects and thus host chains with different number of spins. However, except for the string-order parameter, the measurements that we propose are extremely robust, and in general they produce a signal that is a nonzero average of the possible outcomes for chains of different lengths.

Summing up, in this work we have shown how to implement spin $s = 1$ chains and $s = \frac{1}{2}$ ladders with cold atoms in an optical lattice. Such experiments will allow us to construct never observed phases and probably throw light on the existence of the nematic phase. Finally, we have developed a very general set of tools to characterize these spin phases, which are themselves of interest for future experiments with optical lattices.

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