Three-Spin Interactions in Optical Lattices and Criticality in Cluster Hamiltonians

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We demonstrate that in a triangular configuration of an optical lattice of two atomic species a variety of novel spin-1/2 Hamiltonians can be generated. They include effective three-spin interactions resulting from the possibility of atoms tunneling along two different paths. This motivates the study of ground state properties of various three-spin Hamiltonians in terms of their two-point and n-point correlations as well as the localizable entanglement. We present a Hamiltonian with a finite energy gap above its unique ground state for which the localizable entanglement length diverges for a wide interval of applied external fields, while at the same time the classical correlation length remains finite.

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The combination of cold atom technology with optical lattices [1,2] gives rise to a variety of possibilities for constructing spin Hamiltonians [3,4]. This is particularly appealing as the high degree of isolation from the environment that can be achieved in these systems allows for the study of these Hamiltonians under idealized laboratory conditions. In parallel, techniques have been developed for minimizing imperfections and impurities [5,6] in the implementation of the desired structures and for their subsequent probing and measurement [7]. These achievements permit the experimental investigation of Hamiltonians that are of interest in areas such as quantum information or condensed matter physics with the added advantage of a remarkable freedom in the choice of external parameters. Presently, attention both in condensed matter physics and in cold atom research is focusing on two-spin interactions as these are most readily accessible experimentally. However, the unique experimental capability provided by cold atom technology allows us to relax this restriction. Here we demonstrate that cold atom technology provides a laboratory to generate and study higher order effects such as three-spin interactions that give rise to unique entanglement properties.

The present work serves two purposes. First, it demonstrates that in a two species Bose-Hubbard model in a triangular configuration a wide range of Hamilton operators can be generated that include effective three-spin interactions. They result from the possibility of atomic tunneling through different paths from one vertex to the other. This can be extended to a one-dimensional spin chain with three-spin interactions. Second, we take this novel experimental capability as a motivation to study unique ground state properties of Hamiltonians that include three-spin interactions. In this context one can study possible quantum phase transitions by considering both the classical correlation properties as well as the entanglement properties of these systems. Specifically, we consider the so-called cluster Hamiltonian and its ground state, the cluster state which has previously been shown to play an important role as a resource in the context of quantum computation [8]. Subject to an additional Zeeman term the combined Hamiltonian possesses a finite energy gap above its unique ground state in a finite parameter range, hence exhibiting no critical behavior in the classical correlations in that regime. We shall show that at the same time it exhibits a critical behavior in its entanglement properties due to its three spin-1/2 interaction term. This is manifested by a diverging entanglement length of the localizable entanglement [9]. Our example demonstrates that divergence in entanglement properties are not necessarily related to the existence of classical critical points, the latter giving a rather incomplete description of the long-range quantum correlations against popular belief [10]. A related example was arrived at independently in [11].

Consider an ensemble of ultracold bosonic atoms confined in an optical lattice formed by several standing wave laser beams [3,4,12]. Each atom is assumed to have two relevant internal states, denoted with the index $\sigma = a, b$, which are trapped by independent standing wave laser beams differing in polarization. We are interested in the regime where the atoms are sufficiently cooled and the periodic potential is high enough so that the atoms will be confined to the lowest Bloch band and the low energy evolution can be described by the two species Bose-Hubbard Hamiltonian [12]. The tunneling couplings J^σ and the collisional couplings $U_{\sigma\sigma'}$ can be widely varied by adjusting the amplitude of the lattice laser fields. For the generation of the multiparticle interactions discussed here we require large collisional couplings in order to have a significant effect within the decoherence time of the system. This can be achieved experimentally by Feshbach resonances [13], for which first theoretical [14] and experimental [15] advances are already promising.

Let us begin by considering the case of only three sites in a triangular configuration (see Fig. 1) with tunneling coupling activated between all three of them. We are interested in the regime where the tunneling couplings are much smaller than the collisional ones, $J^\sigma \ll U_{\sigma\sigma'}$

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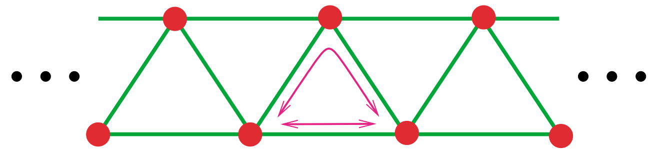

FIG. 1 (color online). The one-dimensional chain constructed out of equilateral triangles. Three-spin interaction terms appear, e.g., between sites i, $i = 1$ and $i + 2$ as, for example, tunneling between i and $i + 2$ can happen through two different paths, directly and through site $i + 1$, the latter resulting into an interaction between i and $i + 2$ that is controlled by the state of site $i + 1$.

which corresponds to the Mott insulating phase and we demand that we have on average one atom per lattice site. Hence, the basis of states of site i can be defined by $|\uparrow\rangle \equiv |n^a = 1, n^b = 0\rangle$ and $|\downarrow\rangle \equiv |n^a = 0, n^b = 1\rangle$, where n^a and n^b are the number of atoms in state a or b, respectively. It is possible to expand the resulting evolution generated by the Bose-Hubbard Hamiltonian in terms of the small parameters $J^\sigma/U_{\sigma\sigma'}$. In an interaction picture with respect to the collisional Hamiltonian, $H^{(0)} = \frac{1}{2}\sum_{i\sigma\sigma'} U_{\sigma\sigma'} a^\dagger_{i\sigma} a^\dagger_{i\sigma'} a_{i\sigma'} a_{i\sigma}$, one obtains the effective evolution from the perturbation expansion up to the third order with respect to the tunneling interaction, $V = -\sum_{i\sigma}(J^\sigma_i a^\dagger_{i\sigma} a_{i+1\sigma} + \text{H.c.})$, given by

$$H = -\sum_\gamma \frac{V_{\alpha\gamma}V_{\gamma\beta}}{E_\gamma} + \sum_{\gamma\delta} \frac{V_{\alpha\gamma}V_{\gamma\delta}V_{\delta\beta}}{E_\gamma E_\delta}. \tag{1}$$

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, E_γ are the eigenvalues of the collisional part, $H^{(0)}$, while we neglected fast rotating terms effective for long time intervals [16]. Written explicitly in terms of spin operators we obtain

$$\begin{aligned} H = \sum_{i=1}^{3} [&\vec{B} \cdot \vec{\sigma}_i + \lambda^{(1)} \sigma^z_i \sigma^z_{i+1} + \lambda^{(2)}(\sigma^x_i \sigma^x_{i+1} + \sigma^y_i \sigma^y_{i+1}) \\ &+ \lambda^{(3)} \sigma^z_i \sigma^z_{i+1} \sigma^z_{i+2} + \lambda^{(4)}(\sigma^x_i \sigma^z_{i+1} \sigma^x_{i+2} \\ &+ \sigma^y_i \sigma^z_{i+1} \sigma^y_{i+2})]. \end{aligned} \tag{2}$$

The couplings $\lambda^{(i)}$ are given as an expansions in $J^\sigma/U_{\sigma\sigma'}$ by

$$\lambda^{(1)} = -\frac{J^{a2}}{U_{aa}} - \frac{9J^{a3}}{2U^2_{aa}} + \frac{J^{a2}}{2U_{ab}} + \frac{J^{a3}}{2U^2_{ab}} + \frac{J^{a3}}{U_{ab}U_{aa}} + (a \leftrightarrow b), \qquad \lambda^{(2)} = -\frac{J^a J^b}{U_{ab}}\left(\frac{1}{2} + \frac{J^a}{U_{aa}} + \frac{3J^a}{2U_{ab}}\right) - \frac{J^{a2}J^b}{2U^2_{aa}} + (a \leftrightarrow b),$$

$$\lambda^{(3)} = -\frac{3J^{a3}}{2U^2_{aa}} + \frac{J^{a3}}{U_{ab}U_{aa}} - (a \leftrightarrow b), \qquad \lambda^{(4)} = -\frac{J^{a2}J^b}{U_{ab}U_{aa}} - \frac{J^{a2}J^b}{2U^2_{aa}} - (a \leftrightarrow b),$$

where the symbol $(a \leftrightarrow b)$ denotes the repeating of the same term as on its left, but with the a and b indices interchanged. The local field $\vec{B}$ can be arbitrarily tuned by applying appropriately detuned laser fields. One can isolate different parts from Eq. (2), each one including a three-spin interaction term, by varying the tunneling and/or the collisional couplings appropriately so that particular $\lambda^{(i)}$ terms such as the two-spin interactions vanish, while others can be varied freely.

In particular, we are interested in obtaining a whole chain of triangles in a zigzag one-dimensional pattern as in Fig. 1. Indeed, with this configuration we can extend from a single triangle to a whole triangular ladder. Nevertheless, a careful consideration of the two spin interactions shows that terms of the form $\sigma^z_i \sigma^z_{i+2}$ also appear, due to the triangular configuration (see Fig. 1). It is possible to introduce a longitudinal optical lattice with half of the initial wave length, and an appropriate amplitude such that it cancels exactly those interactions generating finally chains with only neighboring couplings. With the above procedure we can finally obtain a chain Hamiltonian as in (2) where the summation runs up to the total number N of the sites. A variety of different Hamiltonians could be generated by different combinations of the above techniques.

In the past, Hamiltonians describing three-spin interactions have been of limited interest [17] as they were difficult to implement and control experimentally. The above results demonstrate that Hamiltonians with three-spin interactions can be implemented and controlled across a wide parameter range. One may suspect that ground states of three-spin interaction Hamiltonians exhibit unique properties as compared to ground states generated merely by two-spin interaction. This motivates the study of the properties of the ground state of a particular three-spin Hamiltonian for different parametric regimes. Possible phase transitions induced by varying these parameters are explored employing two possible signatures of critical behavior that are quite different in nature. In particular, new critical phenomena in three-spin Hamiltonians that cannot be detected on the level of classical correlations will be demonstrated.

(i) A traditional approach to criticality of the ground state studies two-point correlation functions between spins 1 and L, given by $C^{\alpha\beta}_{1L} \equiv \langle\sigma^\alpha_1 \sigma^\beta_L\rangle - \langle\sigma^\alpha_1\rangle\langle\sigma^\beta_L\rangle$, for varying L, where $\alpha, \beta = x, y, z$. These two-point correlations may exhibit two types of generic behaviors, namely, (a) exponential decay in L, i.e., the correlation length ξ, defined as

$$\xi^{-1} \equiv \lim_{L\to\infty} \frac{1}{L} \log C^{\alpha\beta}_{1L}, \tag{3}$$

is finite, or (b) power-law decay in L, i.e., $C^{\alpha\beta}_{1L} \sim L^{-q}$ for some q, which implies an infinite correlation length ξ indicating a critical point in the system [10].

(ii) While the two-point correlation functions $C_{1L}^{\alpha\beta}$ are a possible indicator for critical behavior, they provide an incomplete view of the quantum correlations between spins 1 and L. Indeed, they ignore correlations through all the other spins by tracing them out. Already the GHZ state $|\mathrm{GHZ}\rangle = (|000\rangle + |111\rangle)/\sqrt{2}$ shows that this loses important information. Tracing out particle 2 leaves particles 1 and 3 in an unentangled state. However, measuring the second particle in the σ_x eigenbasis leaves particles 1 and 3 in a maximally entangled state. Therefore one may define the localizable entanglement $E_{1L}^{(\mathrm{loc})}$ between spins 1 and L as the largest average entanglement that can be obtained by performing optimized local measurements on all the other spins [9]. In analogy to Eq. (3) one can define the entanglement length

$$\xi_E^{-1} \equiv \lim_{L\to\infty} \frac{1}{L} \log E_{1L}^{(\mathrm{loc})}. \tag{4}$$

It is an interesting question whether criticality according to one of these indicators implies criticality according to the other. The localizable entanglement length is always larger than or equal to the two-point correlation length and indeed, it has been shown that there are cases where criticality behavior can be revealed only by the diverging localizable entanglement length while the classical correlation length remains finite [11]. Such behavior is also expected to appear when we consider particular three-spin interaction Hamiltonians. To see this consider the Hamiltonian

$$H = \sum_i (-\sigma_{i-1}^x \sigma_i^z \sigma_{i+1}^x + B\sigma_i^z), \tag{5}$$

where we assume periodic boundary conditions. The fact that $\sigma_{i-1}^x \sigma_i^z \sigma_{i+1}^x$ commute for different i and employing raising operator $L_k^\dagger = \sigma_k^x - i\sigma_{k-1}^x \sigma_k^y \sigma_{k+1}^x$ allows one to determine the entire spectrum of H for $B = 0$. The unique ground state of H for $B = 0$ is the well-known cluster state [8,18], which has previously been studied as a resource in the context of quantum computation. It possesses a finite energy gap of $\Delta E = 2$ above its ground state [19]. For finite B the energy eigenvalues of the system can still be found using the Jordan-Wigner transformation and a lengthy but straightforward calculation shows that the energy gap persists for $|B| \neq 1$. The exact solution also shows that the system has critical points for $|B| = 1$ at which the two-point correlation length and the entanglement length diverges. For any other value of B and, in particular, for $B = 0$ the system does not exhibit a diverging two-point correlation length as is expected from the finite energy gap above the ground state. Indeed, correlation functions such as

$$C_{1L}^{zz} = \left[\frac{1}{4\pi}\int_{-2\pi}^{2\pi} \frac{\sin r}{\sqrt{B^2+1+2B\cos r}} \sin\frac{(L-1)r}{2} dr\right]^2 - \left[\frac{1}{4\pi}\int_{-2\pi}^{2\pi} \frac{B+\cos r}{\sqrt{B^2+1+2B\cos r}} \cos\frac{(L-1)r}{2} dr\right]^2 \tag{6}$$

can be computed and the corresponding correlation length can be explicitly determined analytically using standard techniques (see, e.g., Fig. 2) [20]. The two-point correlation functions such as Eq. (6) exhibit a power-law decay at the critical points $|B| = 1$ while they decay exponentially for all other values of B in contrast to the anisotropic XY model whose C_{1L}^{xx} correlation function tends to a finite constant in the limit of $L \to \infty$ for $|B| < 1$ [20]. This discrepancy is due to the finite energy gap the model in Eq. (5) exhibits above a nondegenerate ground state in the interval $|B| < 1$.

When we study three-spin interactions it is natural to consider the behavior of higher-order correlations. For the ground state with magnetic field $B = 0$ all three-point correlation except, obviously, $\langle \sigma_{i-1}^x \sigma_i^z \sigma_{i+1}^x \rangle$ vanish. Indeed, if we consider $n > 4$ neighboring sites and chose for each of these randomly one of the operators σ_x, σ_y, σ_z, or $\mathbf{1}$ then the probability that the resulting correlation will be nonvanishing is given by $p = 2^{-(2+n)}$. For $|B| > 0$, however, far more correlations are nonvanishing and the rate of nonvanishing correlations scales approximately as 0.858^n. This marked difference which distinguishes $B = 0$ is due to the higher symmetry that the Hamiltonian exhibits at that point.

In the following we shall consider the localizable entanglement and the corresponding length as described in (ii). Compared to the two-point correlations, the computation of the localizable entanglement is considerably more involved due to the optimization process. Nevertheless, it is easy to show that the entanglement length diverges for $B = 0$. In that case the ground state of the Hamiltonian (5) is a cluster state with the property that any two spins can be made deterministically maximally entangled by measuring the σ_z operator on each spin in between the target spins, while measuring the σ_x operator

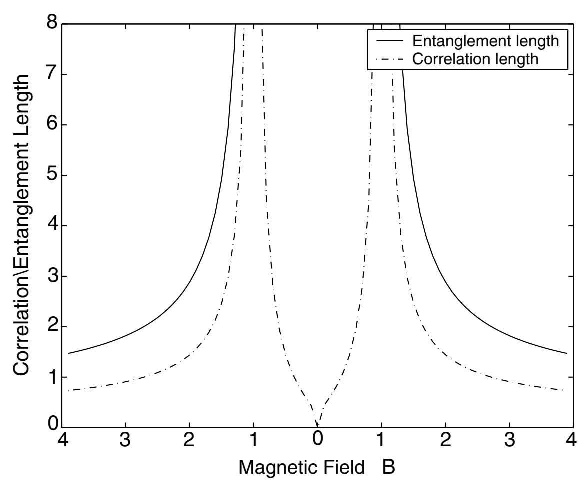

FIG. 2. Both the two-point correlation length for C_{1L}^{zz} (dashed line) and the localizable entanglement length (solid line) are shown for various magnetic field for chain of length 16. Note that the localizable entanglement length diverges in the whole interval $|B| < 1$ while the two-point correlation length is finite in this interval.

on the remaining spins. Indeed, this property underlies its importance for quantum computation as it allows one to propagate a quantum computation through the lattice via local measurements [8].

For finite values of B it is difficult to obtain the exact value of the localizable entanglement. Nevertheless, to establish a diverging entanglement length it is sufficient to provide lower bounds that can be obtained by prescribing specific measurement schemes. Indeed, for the ground state of (5) in the interval $|B| < 1$ consider two spins 1 and $L = 2k + 1$ where $k \in \mathbf{N}$. Measure the σ_x operator on spin 2 and on all remaining spins, other than 1 and L, the σ_z operator. By knowing the analytic form of the ground state one can obtain the average entanglement over all possible measurement outcomes in terms of the concurrence, that tends to $E_\infty = (1 - |B|^2)^{1/4}$ for $k \to \infty$. This demonstrates that the localizable entanglement length is infinite in the full interval $|B| < 1$. This surprising critical behavior for the whole interval $|B| < 1$ is *not* revealed by the two-point or n-point correlation functions which exhibit finite correlation lengths. For $|B| > 1$, however, numerical results, employing a simulated annealing technique to find the optimal measurement for a chain of 16 spins, show that the localizable entanglement exhibits a finite length scale.

In Fig. 2 both the two-point correlation length and localizable entanglement length are drawn versus the magnetic field. In the interval $|B| < 1$ the entanglement length diverges while the correlation length remains finite. For finite temperatures the localizable entanglement becomes finite everywhere but, for temperatures that are much smaller than the gap above the ground state, it remains considerably larger than the classical correlation length. This demonstrates the resilience of this phenomenon against thermal perturbations.

To summarize, we have demonstrated that various Hamiltonians describing three-spin interactions can be created in triangular optical lattices in a two-species Bose-Hubbard model. They can be realized in the laboratory with the near future cold atom technology. In fact, a study of the required experimental values reveals that with a tunneling coupling $J/\hbar \sim 10$ kHz [2] an experimentally achievable collisional coupling of $U/\hbar \sim 100$ kHz is required. A numerical simulation for three sites has been performed for these parameters. It demonstrates that higher-order corrections lead to a 4% renormalization of the coupling strengths in Hamiltonian (2). Note, however, that new interaction terms arise only in 5th order in perturbation due to the triangular geometry of the optical lattice. As a consequence, a significant effect of the three-spin interactions is obtained within the decoherence time of the system taken here to be 10 ms. Previously, the systematic experimental creation of three-spin interaction Hamiltonians has been extremely difficult. The new capability for creation of such Hamiltonians and their possible isolation from other interactions motivates the study of the properties of their ground states and here, in particular, of their phase transitions. Along these lines, we presented a three-spin cluster Hamiltonian that exhibits a novel kind of critical behavior that is not revealed by two-point correlation functions. In addition, interactions such as $\sigma_1^z \sigma_2^z \sigma_3^z$ presented here have proved to be of interest for quantum computation. They can implement multiqubit gates, like the Toffoli gate, in essentially one step [21] reducing dramatically the experimental resources.

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[19] In contrast to Hamiltonian Eq. (5) the two-spin system $H = \sum_i -\sigma_i^x \sigma_{i+1}^x$ does not exhibit a finite gap for an infinite chain and possesses a twofold degenerate ground state. As a consequence the ground state will not be stable [see, e.g., G. Gallavotti, *Statistical Mechanics: A Short Treatise* (Springer, New York, 1999)].

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