Three-spin interactions in optical lattices and criticality in cluster Hamiltonians

Jiannis K. Pachos$^1$ and Martin B. Plenio$^2$

$^1$ Department of Applied Mathematics and Theoretical Physics, University of Cambridge, Cambridge CB3 0WA, UK, $^2$ Quantum Optics and Laser Science Group, Blackett Laboratory, Imperial College, London SW7 2BW, UK.

(Received November 4, 2018)

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.

PACS numbers: 71.10.-w, 03.67.Mn, 03.67.-a

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 idealised laboratory conditions. In parallel, techniques have been developed for minimising 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. Firstly, 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 along different paths from one vertex to the other. This can be extended to a one dimensional spin chain with three-spin interactions. Secondly, 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 [20]. 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 behaviour in the classical correlations in that regime. We shall show that at the same time it exhibits a critical behaviour 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 [8]. 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 [9]. A related example was arrived at independently in [10].

Consider an ensemble of ultracold bosonic atoms confined in an optical lattice formed by several standing wave laser beams [3,4,11]. 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 polarisation. 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 [11]. The tunneling couplings $J^\sigma$ 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 multi-particle 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 [12–14], for which first theoretical [15] and experimental [16] advances are already promising.

Let us begin by considering the case of only three sites in a triangular configuration (see Figure 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, $J^\sigma \ll U_{\sigma\sigma'}$ 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
\[ |\downarrow\rangle \equiv |n^a = 0, n^b = 1\rangle, \text{ where } n^a \text{ and } n^b \text{ are the number of atoms in state } a \text{ or } b \text{ respectively. It is possible to expand the}\]
\[ \text{the effective evolution from the perturbation expansion up to the third order with respect to the tunneling interaction, } V = -\sum_\alpha \langle \hat{J}_\alpha^a a^\dagger_{\alpha i} a^\dagger_{\alpha (i+1)+} + H.c.\rangle, \text{ given by}\]
\[ H = -\sum_\gamma V_{\gamma\gamma} V_{\gamma\beta}/E_{\gamma} + \sum_\gamma V_{\gamma\gamma} V_{\gamma\beta}/E_{\gamma} E_{\delta}. \] (1)

The indices \( \alpha, \beta \) refer to states with one atom per site while \( \gamma, \delta \) refer to states with two or more atomic populations per site, \( E_{\gamma} \) are the eigenvalues of the collisional part, \( H^{(0)} \), while we neglected fast rotating terms effective for long time intervals [17]. Written explicitly in terms of spin operators we obtain
\[ H = \sum_{i=1}^3 \tilde{B} \cdot \hat{\sigma}_i + \lambda(1)\sigma^z_i \sigma^z_{i+1} + \lambda(2)(\sigma^x_i \sigma^x_{i+1} + \sigma^y_i \sigma^y_{i+1}) \]
\[ + \lambda(3)\sigma^z_i \sigma^z_{i+1} \sigma^z_{i+2} + \lambda(4)(\sigma^x_i \sigma^x_{i+1} \sigma^x_{i+2} + \sigma^y_i \sigma^y_{i+1} \sigma^y_{i+2}). \] (2)

The couplings \( \lambda^{(i)} \) are given as expansions in \( J^\sigma/U_{\sigma\sigma} \) by
\[ \lambda^{(1)} = -\frac{J^a_a}{U_{aa}} - \frac{J^b_b}{U_{bb}} - \frac{3}{2} \frac{J^a_a}{U_{aa}^2} - \frac{3}{2} \frac{J^b_b}{U_{bb}^2} + \frac{1}{2} \frac{J^a_a + J^b_b}{U_{ab}} \]
\[ + \frac{1}{2} \frac{J^a_a + J^b_b}{U_{ab}^2} \frac{J^a_a}{U_{aa}} + \frac{J^b_b}{U_{bb}} + \frac{1}{2} \frac{J^a_a}{U_{aa}} \frac{J^b_b}{U_{bb}} + \lambda^{(2)} \]
\[ \lambda^{(2)} = -\frac{J^a_a}{U_{ab}} (1 + \frac{J^a_a}{U_{aa}} + \frac{J^b_b}{U_{bb}} + \frac{3}{2} \frac{J^a_a}{U_{ab}} + \frac{J^b_b}{U_{ab}}) \]
\[ - \frac{1}{2} \frac{J^a_a}{U_{ab}^2} + \frac{J^b_b}{U_{bb}} \frac{J^a_a}{U_{aa}} + \frac{J^b_b}{U_{bb}} \frac{J^a_a}{U_{ab}} \]
\[ \lambda^{(3)} = -\frac{3}{2} \frac{J^a_a}{U_{ab}^2} \frac{J^a_a}{U_{aa}} + \frac{J^b_b}{U_{bb}} \frac{J^a_a}{U_{ab}} + \frac{1}{2} \frac{J^a_a}{U_{ab}} \frac{J^b_b}{U_{bb}} + \lambda^{(4)} \]
\[ \lambda^{(4)} = -\frac{J^a_a}{U_{ab}} (1 + \frac{J^a_a}{U_{aa}} + \frac{J^b_b}{U_{bb}} + \frac{3}{2} \frac{J^a_a}{U_{ab}} + \frac{J^b_b}{U_{ab}}) \]
\[ - \frac{1}{2} \frac{J^a_a}{U_{ab}^2} + \frac{J^b_b}{U_{bb}} \frac{J^a_a}{U_{aa}} + \frac{J^b_b}{U_{bb}} \frac{J^a_a}{U_{ab}} \]

The local field \( \tilde{B} \) can be arbitrarily tuned by applying appropriately detuned laser fields while we need to compensate for single particle phase rotations of the form \( B_z \sum_\alpha \sigma^z_\alpha \) with
\[ B_z = -\frac{J^a_a}{U_{aa}} (2 + \frac{9}{2} \frac{J^a_a}{U_{aa}} + \frac{J^a_a}{U_{bb}}) + \frac{J^b_b}{U_{bb}} (2 + \frac{9}{2} \frac{J^b_b}{U_{bb}} + \frac{J^b_b}{U_{aa}}) \] (3)

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.

By employing additional Raman transitions in such a way as to couple the states \( a \) and \( b \) during tunneling it is possible to obtain variations of the above Hamiltonian [4]. Indeed, Raman transitions can activate tunneling of the states \( |\downarrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) \), while the tunneling of the states \( |\uparrow\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle) \) is obstructed. Hence, it is possible to generate different coefficients in front of the two spin interaction terms \( \sigma^z_i \sigma^z_{i+1} \) or \( \sigma^y_i \sigma^y_{i+1} \) as they are the diagonal matrices in their corresponding basis \( |\downarrow\rangle \) or \( |\uparrow\rangle \). Considering its effect on the three-spin interaction it is possible to generate additional terms of the form \( \sigma^z_i \sigma^z_{i+1} \sigma^z_{i+2} \) or \( \sigma^y_i \sigma^y_{i+1} \sigma^y_{i+2} \) with couplings similar to \( \lambda^{(3)} \). Note that the effective spin interactions produced by Raman transitions do not preserve the number of particles in each of the species.

In particular, we are interested in obtaining a whole chain of triangles in a zig-zag 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). Hamiltonians involving nearest and next-to-nearest neighbour interactions are of interest in their own right (see e.g. Chapter 14 of [9] and [18]), but we will not address these systems here. 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 neighbouring couplings.

![FIG. 1. 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 \( i+1 \).](image-url)
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 behaviour 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 \( C_{1L}^{\alpha \beta} \equiv \langle \sigma_1^\alpha \sigma_L^\beta \rangle - \langle \sigma_1^\alpha \rangle \langle \sigma_L^\beta \rangle \), for varying \( L \), where \( \alpha, \beta = x, y, z \). These two-point correlations may exhibit two types of generic behaviours, namely (a) exponential decay in \( L \), i.e. the correlation length \( \xi \), defined as

\[
\xi^{-1} \equiv \lim_{L \to \infty} \frac{1}{L} \log C_{1L}^{\alpha \beta}, \tag{3}
\]

is finite or, (b), power-law decay in \( L \), i.e. \( C_{1L}^{\alpha \beta} \sim L^{-q} \) for some \( q \), which implies an infinite correlation length \( \xi \) indicating a critical point in the system [9].

(ii) While the two-point correlation functions \( C_{1L}^{\alpha \beta} \) are a possible indicator for critical behaviour, 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 \( |GHZ\rangle = (|000\rangle + |111\rangle)/\sqrt{2} \) shows that this looses important information. Tracing out particle 2 leaves particles 1 and 3 in an unentangled state. However, measuring the second particle in the \( \sigma_z \)-eigenbasis leaves particles 1 and 3 in a maximally entangled state. Therefore one may define the localizable entanglement \( E_{1L}^{(loc)} \) between spins 1 and \( L \) as the largest average entanglement that can be obtained by performing optimised local measurements on all the other spins [8]. In analogy to Eq. (3) one can define the entanglement length

\[
\xi_{E}^{-1} \equiv \lim_{L \to \infty} \frac{1}{L} \log E_{1L}^{(loc)}. \tag{4}
\]

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 behaviour can be revealed only by the diverging localizable entanglement length while the classical correlation length remains finite [10]. Such behaviour is also expected to appear when we consider particular three-spin interaction Hamiltonians. To see this consider the Hamiltonian

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

where we assume periodic boundary conditions. The fact that \( \sigma_{i-1}^x \sigma_i^z \sigma_{i+1}^z \) commute for different \( i \) and employing raising operator \( L_k^i = \sigma_k^z - i \sigma_{k-1}^y \sigma_{k+1}^y \) allows 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 [20,21], 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 [22]. 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

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

can be computed and the corresponding correlation length can be explicitly determined analytically using standard techniques (see e.g. Fig. (2)) [23]. 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 \( C_{1L}^{zz} \) correlation function tends to a finite constant in the limit of \( L \to \infty \) for \( |B| < 1 \) [23]. This discrepancy is due to the finite energy gap the model in Eq. (5) exhibits above a non-degenerate ground state in the interval \( |B| < 1 \).

When we study three-spin interactions it is natural to consider the behaviour of higher-order correlations. For the ground state with magnetic field \( B = 0 \) all three-point correlation except, obviously, \( \langle \sigma_{i-1}^x \sigma_i^y \sigma_{i+1}^z \rangle \) vanish. Indeed, if we consider \( n > 4 \) neighbouring sites and chose for each of these randomly one of the operators \( \sigma_x, \sigma_y, \sigma_z \) or 1 then the probability that the resulting correlation will be non-vanishing is given by \( p = 2^{-2n}\). For \( |B| > 0 \) however far more correlations are non-vanishing and the rate of non-vanishing 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 \( \sigma_z \) operator on each
spin in between the target spins, while measuring the $\sigma_z$ operator on the remaining spins. Indeed, this property underlies its importance for quantum computation as it allows to propagate a quantum computation through the lattice via local measurements [20].

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 $k \in \mathbb{N}$. Measure the $\sigma_z$ operator on spin 2 and on all remaining spins, other than 1 and $L$, the $\sigma_z$ 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 behaviour for the whole interval $|B| < 1$ is not revealed by the two-point or n-point correlation function 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.

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. With these values a full numerical study demonstrates that the perturbative truncation is valid within a 4% error and a significant effect of the three spin interactions is obtained within the decoherence time of the system taken here to be 10ms. Previously, the systematic experimental creation of three-spin interaction Hamiltonians has been extremely difficult. The new capability for the systematic creation of three-spin 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. Motivated by this we presented a particular 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 multi-qubit gates, like the Toffoli gate, in essentially one step [24] reducing dramatically the experimental resources.

Acknowledgements. We thank Derek Lee for inspiring conversations. This work was supported by a Royal Society University Research Fellowship, a Royal Society Leverhulme Trust Senior Research Fellowship, the EU Thematic Network QUPRODIS and the QIP-IRC of EPSRC.

![FIG. 2](image-url)  
**FIG. 2.** Both, the two-point correlation length for $C_{zz}^{(2)}$ (solid line) and the localizable entanglement length (dashed 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.

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.

[1] A. Kastberg, et. al., Phys. Rev. Lett. 74, 1542 (1995); G. Raithel, et. al., Phys. Rev. Lett. 81, 3615 (1998).
[2] M. Greiner, et. al., Nature 415, 39 (2002); M. Greiner, et. al., ibid 419, 51 (2002); O. Mandel, et. al., ibid 425, 937 (2003).
[3] A. B. Kuklov and B. V. Svistunov, Phys. Rev. Lett. 90, 100401 (2003).
[4] L.-M. Duan, et. al., Phys. Rev. Lett. 91, 090402 (2003).
[5] P. Rabl et al, cond-mat/0304026.
[6] S. E. Sklarz, et. al., Phys. Rev. A 66, 053620 (2002).
[7] D. C. Roberts and K. Burnett, Phys. Rev. Lett. 90, 150401 (2003).
[8] F. Verstraete, et. al., Phys. Rev. Lett. 92, 027901 (2004).
[9] S. Sachdev, Quantum Phase Transitions, Cambridge University Press (1999).
[10] F. Verstraete, et. al., Phys. Rev. Lett. 92, 087201 (2004).
[11] D. Jaksch, et. al., Phys. Rev. Lett. 81, 3108 (1998).
[12] S. Inouye, et. al., Nature 392, 151 (1998).
[13] A. Donley, et. al., Nature 412, 295 (2001).
[14] S. J. J. M. F. Kokkelmans, and M. J. Holland, Phys. Rev. Lett. 89, 180401 (2002); T. Koehler, T. Gasenzer, and K. Burnett, cond-mat/0209100.
[15] F. H. Mies, et. al., Phys. Rev. A 61, 022721 (2000).
[16] E. A. Donley, et. al., Nature (London) 417, 529 (2002).
[17] J. K. Pachos and E. Rico, quant-ph/0404048.
[18] P. Fendley, et. al., Phys. Rev. B 69, 075106 (2004).
[19] K. A. Penson, et. al., Phys. Rev. B 26, 6334 (1982); K. A. Penson, et. al., Phys. Rev. B 37, 7884 (1988); J. C. A. d’Auria, and F. Iglói, Phys. Rev. E 58, 241 (1998).
[20] R. Raussendorf, et. al., Phys. Rev. A 68, 022312 (2003).
[21] F. Verstraete, and J. I. Cirac, quant-ph/0311130.
[22] In contrast to Hamiltonian Eq. (5) the two-spin system \( H = \sum_{i} -\sigma_{i}^{z}\sigma_{i+1}^{z} \) does not exhibit a finite gap for an infinite chain and possesses a two-fold degenerate ground state. As a consequence the ground state will not be stable (see eg G. Gallavotti, Statistical Mechanics: A Short Treatise, Springer 1999).
[23] E. Barouch and B. M. McCoy, Phys. Rev. A 3, 786 (1971).
[24] J. K. Pachos and P. L. Knight, Phys. Rev. Lett. 91, 107902 (2003).