Sharp Phase Transitions in a Small Frustrated Network of Trapped Ion Spins

G.-D. Lin, C. Monroe, and L.-M. Duan

Phys. Rev. Lett. **106**, 230402 — Published 8 June 2011

DOI: 10.1103/PhysRevLett.106.230402

Sharp phase transitions in a small frustrated network of trapped ion spins

G.-D. Lin[1], C. Monroe[2], and L.-M. Duan[1]
[1]*Department of Physics and MCTP, University of Michigan, Ann Arbor, Michigan 48109*
[2]*Joint Quantum Institute, University of Maryland Department of Physics and National Institute of Standards and Technology, College Park, MD 20742*

Sharp quantum phase transitions typically require a large system with many particles. Here we show that for a frustrated fully-connected Ising spin network represented by trapped atomic ions, the competition between different spin orders leads to rich phase transitions whose sharpness scales exponentially with the number of spins. This unusual finite-size scaling behavior opens up the possibility of observing sharp quantum phase transitions in a system of just a few trapped ion spins.

PACS numbers: 03.67.Lx, 37.10.Ty, 05.30.Rt, 75.10.Jm

Quantum simulators are motivated by the promise of gaining insight into many-body quantum systems such as high-T_C superconductors or complex arrangements of interacting spins. Cold atomic systems form a promising platform for quantum simulation, as the interactions between particles can be under great control. A good example is a collection of trapped and laser-cooled atomic ions, each representing an effective spin that can be made to interact with all the others by modulating the Coulomb interaction between ions. By applying spin-dependent optical dipole forces it has been shown that a crystal of ions provides an ideal platform to simulate intractable interacting spin models [1, 2]. Following this proposal, recent experiments have simulated quantum magnetism with a few ions [3–6]. For three or more ions, the long-range coupling between the spins can provide frustrated interaction patterns or competition between various spin orders and offer an exceptional opportunity to study quantum phases and transitions [5, 6]. A quantum phase transition is defined as a singular change of the ground state energy as one continuously varies a control parameter in the Hamiltonian, characterized by a level crossing or an avoid level crossing that approaches a singularity as the system size increases [7]. The observation of a quantum phase transition typically requires a large system with many particles, as the width (sharpness) of a quantum phase transition usually scales with $1/N$, the inverse of the number of particles [7]. With such slow finite-size scaling laws, small networks of trapped ions realized in current experiments ($N \lesssim 20$) are not expected to exhibit sharp transitions between distinct quantum phases.

In this paper, we show the surprising result that sharp phase transitions can indeed be observed with just a few atomic ions. This is due to unusual finite size scaling laws in this frustrated spin network, where the sharpness of some phase transitions scales exponentially instead of linearly with $1/N$. By controlling a single experimental parameter that determines the pattern of spin-spin couplings between the ions, we show that the expected ground state emerges from a delicate compromise between the couplings. Frustration in the spin network leads to a variety of spin orders, with the number of distinct phases increasing rapidly with the number of ions. We construct the complete phase diagram for small spin networks realizable with the current technology. The sharp phase transition is characterized in detail with an explanation of its unusual finite-size scaling behavior.

We consider a small crystal of ions confined in a one-dimensional harmonic trap. The spin states of the ions are represented by two internal states, referred as $|\uparrow\rangle$ and $|\downarrow\rangle$, and the effective spin-spin interaction between the ions is induced with off-resonant bichromatic laser beams [1, 3–5]. The ion-laser coupling Hamiltonian, written in the rotating frame, has the form $H = \sum_n [\hbar\Omega\cos(\delta k x_n + \mu t)\sigma_n^z + B\sigma_n^x]$ [8], where Ω is a Raman Rabi frequency, δk is the wave vector difference between the two Raman beams (which is assumed to be along the radial direction $\hat{x}$), μ is the beatnote or detuning between the two laser beams, σ_n^z and σ_n^x are Pauli matrices describing the spin of the nth ion, and B is an effective magnetic field induced by radiation that coherently flips the spins. In the rotating frame, the radial coordinate x_n is expanded in terms of the transverse phonon modes a_k as $x_n = \sum_k b_n^k \sqrt{\hbar/(2m\omega_k)}(a_k^\dagger e^{i\omega_k t} + a_k e^{-i\omega_k t})$, where m is the atomic mass, ω_k is the eigenfrequency of the kth normal mode of the ion crystal, and b_n^k is the eigenmode transformation matrix. We use transverse phonon modes because they can more easily be scaled up to large systems [5, 9]. Under the Lamb-Dicke criterion $\eta_{n,k} \equiv b_n^k \delta k \sqrt{\hbar/(2m\omega_k)} \ll 1$, the Hamiltonian H is simplified to $H = -\hbar\Omega\sum_{nk}\eta_{n,k}\sin(\mu t)\,\sigma_n^z(a_k^\dagger e^{i\omega_k t} + a_k e^{-i\omega_k t}) + B\sum_n \sigma_n^x$.

If we assume that the laser detuning μ is not resonant with any phonon mode with the condition $|\omega_k - \mu| \gg \eta_{n,k}\Omega$ satisfied for all n modes k, the probability of exciting any phonon mode $\left|\Omega\eta_{n,k}b_n^k/2\,(\omega_k - \mu)\right|^2$ is negligible. We can therefore adiabatically eliminate the phonon modes and arrive at the following effective spin-spin coupling Hamiltonian [6, 10]

$$H_s = \sum_{m,n} J_{mn}\sigma_m^z\sigma_n^z + B\sum_n \sigma_n^x, \tag{1}$$

where the coefficients

$$J_{mn} = \frac{(\hbar\Omega\delta k)^2}{2m}\sum_k \frac{b_m^k b_n^k}{\mu^2 - \omega_k^2}. \tag{2}$$

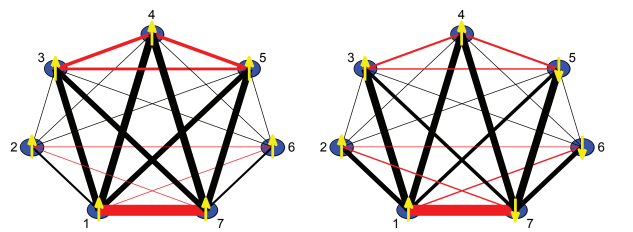

Figure 1: (Color online) Illustration of spin orders in two frustrated Ising networks with competing long-range interaction for $N = 7$ ions. *Left panel*: Ferromagnetic order with detuning $\mu/\omega_\perp = 0.9886$; *Right panel*: Kink order with $\mu/\omega_\perp = 0.9900$. The thickness of the edge in the graph represents the strength of each coupling. Positive (antiferromagnetic) spin couplings are indicated in red, while negative (ferromagnetic) couplings are indicated in black. (Throughout this paper, we set the trap aspect ratio (transverse/axial) $\omega_\perp/\omega_\parallel = 10$ [4–6].)

This Ising Hamiltonian is a pillar of many-body physics, and its properties have been exhaustively studied under various conditions [7]. For instance, the ground state of the Ising Hamiltonian is well understood when the coupling coefficients J_{mn} are uniform, or nonzero only for nearest neighbors. However, here we have an extended Ising network where the coupling coefficients J_{mn} are inhomogeneous (both in magnitude and sign) and extend over long range [11]. The strong competition among these interaction terms (even with $B = 0$) will generally lead to highly frustrated ground states where individual bonds are compromised in order to reach a global energy minimum. For arbitrary coupling coefficients J_{mn}, the determination of the ground state energy of Hamiltonian (1) generally belongs to the complexity class of NP-complete problems [12], meaning that calculating attributes of the system becomes intractable when the system size is scaled up.

We consider the case where the coupling coefficients J_{mn} are controlled by a single experimental parameter, the laser detuning μ [4–6]. To determine J_{mn} from detuning μ with the formula (2), we need the normal mode eigenfunction b_n^k. This is obtained by finding the equilibrium positions for a given number of ions in a harmonic trap and then diagonalizing the Coulomb interaction Hamiltonian expanded around the ions' equilibrium positions. With a single control parameter μ, we are not able to program arbitrary coupling coefficients J_{mn}. However, the interaction pattern is sufficiently complex to allow frustrated ground state configurations and rich phase transitions. To illustrate this, we show in Fig. 1a coupling pattern for $N = 7$ ions and its associated ground state spin configuration at $B = 0$. The coupling pattern is represented by a graph where the color and the thickness of each edge represents respectively the sign (ferromagnetic or antiferromagnetic) and the magnitude of the coupling. In Fig. 1a, we find a ferromagnetically ordered ground state with all the spins pointing to the same direction. However, in this ferromagnetic state, some of the bonds, such as the strong antiferromagnetic bond between the ions 1 and 7, are compromised, and due to this frustration, the ground-state spin configuration is very sensitive to the strength of the coupling. If we adjust the detuning μ by a small fraction of the trap frequency, the ferromagnetic bonds of the ion pairs $(1, 5)$ and $(3, 7)$ are slightly weakened (see Fig. 1b) and the antiferromagnetic bond $(1, 7)$ dominates and flips the spin direction of the entire left (or right) half of the ion crystal. This is a phase transition from ferromagnetic order to a "kink" order, with a kink in the spin direction between the 4th and 5th ions counting from either the left or the right side.

To show the rich phase diagram for this system, in Fig. 2a we list all different spin phases at $B = 0$ for a small Ising network with 3, 5, 7 and 9 ions obtained through exact diagonalization of the Hamiltonian while tuning up the detuning μ. For an odd number of ions, the phase diagram is more interesting and features a larger variety of spin orders, because the left-right reflection symmetry in a linear ion crystal can be spontaneously broken. Each phase is characterized by a spin order (denoted with a binary string where 0 and 1 correspond to $\uparrow$ and $\downarrow$ spin respectively) which gives one of the ground state spin configurations. The Ising Hamiltonian (1) features a reflection symmetry and an intrinsic Z_2 symmetry with respect to a global spin flip. The spin order breaks the Ising symmetry, so each phase is at least two-fold degenerate. If the spin order also breaks the reflection symmetry, the corresponding ground state is 4-fold degenerate. For instance, for the phase denoted by the spin order 01001, the four degenerate ground states are $|\downarrow\uparrow\downarrow\downarrow\uparrow\rangle$, $|\uparrow\downarrow\uparrow\uparrow\downarrow\rangle$, $|\uparrow\downarrow\downarrow\uparrow\downarrow\rangle$, and $|\downarrow\uparrow\uparrow\downarrow\uparrow\rangle$. When μ is tuned crossing a phonon mode (numbers in parentheses in Fig. 2a), the spin order changes as expected, but this is not a conventional phase transition as the parameters J_{mn} change discontinuously in the Hamiltonian (1). However, when μ varies within two phonon modes, all the parameters J_{mn} are analytic functions of μ, yet the spin order can still change abruptly, signaling a phase transition. The frequency of this type of inter-mode phase transition increases rapidly with the ion number: there is one such transition for a three-ion chain and 12 such transitions in a nine-ion crystal. Another notable feature from Fig. 2a is that there is typically no phase transition when μ varies from an even mode (2nd, 4th, ..., phonon modes; counting from the lowest phonon frequency) to an odd mode (3rd, 5th, ...). In such regions, the spin order has a reflection symmetry. This suggests that a spin order with reflection symmetry may be more stable in energy and does not easily yield to other spin configurations. This observation is consistent with the fact that for an even number of ions, there are much fewer inter-mode phase transitions, as the spin order in these cases has a reflection symmetry.

As we add a transverse B field to the Hamiltonian, the spins will gradually become polarized along the x-direction along B. In Fig. 2b, we plot the average polarization $\langle \sum_n \sigma_n^x \rangle / N$ as a function of the field

(a)

$N=3$ Spin order	Trans. Pt.
010	
	(0.9879)
000	
	0.9911
001	
	(0.9950)
000	
	(1)
010	

$N=5$ Spin order	Trans. Pt.
01010	
	(0.9683)
00000	
	0.9691
00001	
	0.9702
00110	
	0.9708
01001	
	(0.9789)
01110	
	(0.9879)
00000	
	0.9897
00011	
	(0.9950)
00000	
	(1)
01010	

$N=7$ Spin order	Trans. Pt.
0101010	
	(0.94166)
0000000	
	0.94176
0000001	
	0.94198
0111110	
	0.94223
0100110	
	0.94454
0100101	
	(0.95572)
0100010	
	(0.96812)
0000000	
	0.96813
0001110	
	0.96934
0110001	
	(0.97885)
0111110	
	(0.98785)
0000000	
	0.98916
0000111	
	(0.99499)
0000000	
	(1)
0101010	

$N=9$ Spin order	Trans. Pt.
010101010	
	(0.907860)
000000000	
	0.907868
000000001	
	0.907886
011111110	
	0.907918
010011010	
	0.910853
010100101	
	(0.925439)
010111010	
	(0.941301)
000000000	
	0.941406
000011100	
	0.941816
001100010	
	0.942805
010001101	
	(0.955478)
011000110	
	(0.967979)
000000000	
	0.967986
010100001	
	0.968032
011010001	
	0.968212
(continued)	
000011110	
	0.968507
011100001	
	(0.978784)
001111100	
	(0.987832)
000000000	
	0.988824
000001111	
	(0.994987)
000000000	
	(1)
010101010	

unit : $\omega_\perp$ ($\omega_\perp/\omega_\parallel = 10$)

(b)

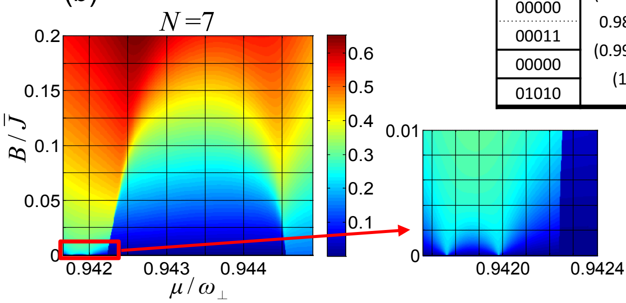

Figure 2: (Color online) (a) Ground-state phases at $B=0$ characterized by the corresponding spin orders for $N=3,5,7,9$ ions. The transition points are positioned by the values of μ whereas the phonon mode frequencies are presented in parentheses. (b) Average polarization $\langle\Psi_G|\sum_n\sigma_n^x|\Psi_G\rangle/N$ for $N=7$ ions at finite fields B with $|\Psi_G\rangle$ denoting the ground state. The right figure is a closeup near the critical point.

B (in the unit of the average J_{mn} defined by $\bar{J}\equiv\sqrt{\sum_{m\neq n}|J_{mn}|^2/[N(N-1)]}$) for $N=7$ ions in a small region of the detuning μ. We find that the system is easily polarized if it lies at the critical point between two different spin orders given by the Ising couplings. But near the center of a spin phase, the spin order is more robust and can persist under a finite B, eventually yielding to the polarized phase as B increases through the Ising-type transition (which becomes a broad crossover for this finite system).

With $B=0$, the transition between different spin orders is sharp as it is characterized by a level crossing for the ground state of the Hamiltonian (1). When we turn on a finite B field, the system shows only avoided level crossings in its ground state, and typically the sharp phase transition at $B=0$ should be replaced by a broad crossover for this small system, similar to the Ising-type of transition discussed above. Interestingly, this is not always the case. We find that for some transition, even at a finite B, the boundary between different spin phases remains very sharp (as characterized by the transition width defined in Fig. 4). To see this clearly, we look at a particular example: for N ions when N is odd [13], numerical diagonalization shows there is a unique spin phase transition in the region between the 2nd and 3rd highest modes. A schematic phase diagram for this region is presented in Fig. 3a. At $B=0$, we have a ferromagnetic phase on the left side which is doubly degenerated and a kink phase on the right side which is 4-fold degenerate. At finite B, these two spin orders remain robust in a range of B, before eventually yielding to a polarized phase for a large B field through a crossover. In Fig. 3b and 3c, the transition between the ferromagnetic (red region) and the kink (blue region) phases can be witnessed by the emergence of the sharp boundary when the number of particles is moderately increased from 5 to 9. It is also interesting to note that the transition boundary between these two phases has a slope with the B axis, so one can cross this phase transition by tuning either the detuning μ or the field B.

To characterize sharpness of the transition between the ferromagnetic phase and the kink phase, in Fig. 4a we look at energies of the four lowest eigenstates of the Hamiltonian (1) as functions of B or μ across the phase boundary. While the ground state energy is a smooth function of μ at a finite B, the first and second excited states have a level crossing. As the number of ions N increases, the ground state energy quickly approaches the level crossing point with the energy gap ΔE shown in Fig. 4a shrinking exponentially with N, signaling a sharp phase transition already at a modest ion number. The transition width W defined in Fig. 4 is apparently proportional to the energy gap ΔE, and in Fig. 4b, ΔE is shown as a function of the ion number N, which can be well fit with the formula $\Delta E\simeq\bar{J}(B/\bar{J})^{(N-1)/2}$. The exponential shrinking of ΔE with N can be intuitively understood as follows: when $B\ll\bar{J}$ we can treat the term $B\sum_n\sigma_n^x$ as a perturbation in the Hamiltonian (1). For each application of $B\sum_n\sigma_n^x$, we can only flip the direction of one spin. As the ferromagnetic state and the kink state have $(N-1)/2$ spins taking opposite directions, the two states need to be connected through $(N-1)/2$-th order perturbation, and thus the energy gap is proportional to $(B/\bar{J})^{(N-1)/2}$.

As one can see from Fig. 2a, the typical spacings between the transverse modes are very insensitive to the ion number N under a fixed aspect ratio $\omega_\perp/\omega_{||}$ that is large

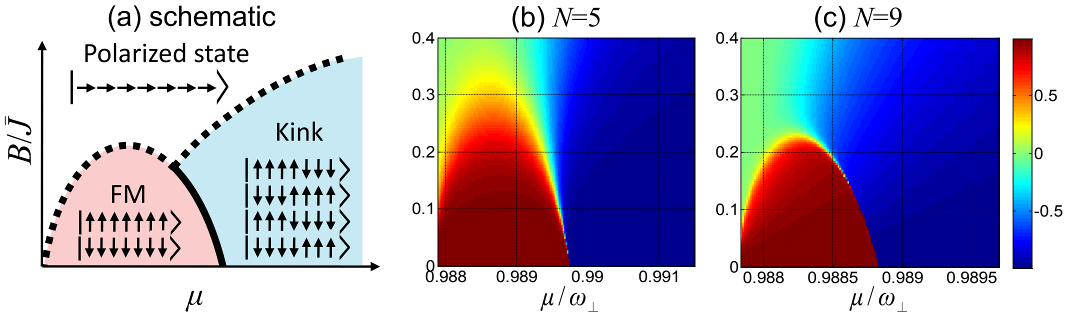

Figure 3: (Color online) (a) The schematic phase diagrams for odd numbers of ions in the region between the 2nd and 3rd highest modes. For a small number of ions, the solid line represents a sharp transition, whereas the dashed lines represent a continuous crossover to the polarized state. (b,c) The calculated theoretical phase diagrams for (b) $N = 5$ and (c) $N = 9$ ions. Color shows the order parameter defined by $P_{FM} - P_K$, where $P_{FM} \equiv \sum_{s=\uparrow,\downarrow} |\langle s, s, \cdots, s|\Psi_G\rangle|^2$ and $P_K \equiv \sum_{s=\uparrow,\downarrow} |\langle s^{(\frac{N+1}{2})}, \bar{s}^{(\frac{N-1}{2})}|\Psi_G\rangle|^2 + |\langle s^{(\frac{N-1}{2})}, \bar{s}^{(\frac{N+1}{2})}|\Psi_G\rangle|^2$ are the projection probabilities of the ground state $|\Psi_G\rangle$ of the system to the Hilbert subspace with the ferromagnetic and the kink orders, respectively. ($|s^{(m)}, \bar{s}^{(N-m)}\rangle \equiv \Pi_{i=1}^{m}|s_i\rangle\Pi_{i=m+1}^{N}|\bar{s}_i\rangle$, where s denotes the spin orientation with $\bar{\uparrow} \equiv\downarrow$ and vice versa).

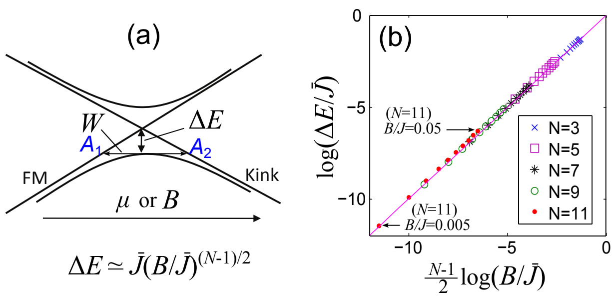

Figure 4: (a) The structure of the lowest four energy levels around the sharp ferromagnetic-kink phase transition. The two lowest states have a ferromagnetic (kink) order on the left (right) side. The transition width W is defined as the distance between two points A_1 and A_2 located in the ferromagnetic (kink) phase, respectively, with the order parameter $P_{FM} - P_K$ defined in Fig. 3 caption changing from 0.71 (at A_1) to -0.68 (at A_2) for $N = 9$ and $B/\bar{J} = 0.05$. (b) Data points ΔE (in log-scale) as a function of the ion number N and magnetic field B, on top of a solid line representing the relation $\kappa \equiv \log(\Delta E/\bar{J})/[\frac{N-1}{2}\log(B/\bar{J})] = 1$. For each N, those dots correspond to $B/\bar{J}$ increasing from 0.005 to 0.05 with a step-size of 0.005. The largest deviation in this figure occurs at $N = 11$, $B/\bar{J} = 0.05$, where $\kappa - 1 = 3.4\%$.

enough to stabilize the ion chain. For instance, the spacing between the highest and the second highest modes can be roughly estimated by $\delta\omega_{12} \simeq \omega_{||}^2/(2\omega_\perp)$, which is clearly independent of N. To observe the sharp phase transition predicted in Fig. 3, we need a resolution in detuning μ about the order of $\sim 5 \times 10^{-4}\omega_\perp = 2.5$ kHz under a typical value of $\omega_\perp \sim 2\pi \times 5$ MHz. This is feasible with current technology where the detuning can be controlled very precisely. The width of transition defined in Fig. 4 shrinks very rapidly with N: for instance, with $N = 9$ and $B/\bar{J} = 0.05$, the width has been reduced to $W \sim 3 \times 10^{-6}\delta\omega_{12}$, so it is possible to observe a very sharp phase transition with a few ions already.

In summary, we have shown that laser induced magnetic coupling between trapped ions realizes a frustrated Ising spin network with competing long range interactions, giving rise to rich phase diagrams for the ground state. Some of the phase transitions in this system are characterized by a unusual finite size scaling, where the transition width scales down exponentially with the number of ions. This exponential finite size scaling leads to sharp phase transitions for a small system even with just a few ions, as one can realize now in the lab.

This work was supported by the DARPA OLE program, the IARPA MQCO program, the AFOSR and the ARO MURI programs, the NSF PIF Program, and the NSF Center at JQI.

[1] D. Porras and J. I. Cirac, Phys. Rev. Lett. 92, 207901 (2004).

[2] X.-L. Deng, D. Porras, and J. I. Cirac, Phys. Rev. A 72, 063407 (2005).

[3] A. Friedenauer et al., Nature Physics 4, 757 (2008).

[4] K. Kim et al., Phys. Rev. Lett. 103, 120502 (2009).

[5] K. Kim et al., Nature 465, 590-593 (2010).

[6] E. E. Edwards et al., Phys. Rev. B 82, 060412 (2010).

[7] S. Sachdev, Quantum Phase Transitions, Cambridge University Press, Cambridge (1999); P. Ribeiro, J. Vidal, and R. Mosseri, Phys. Rev. E 78, 021106 (2008).

[8] In the experiments of Refs. [4-6], the lasers drive a σ_n^x-dependent force (see A. Sorensen and K. Molmer, Phys. Rev. A 62, 022311 (2000).) Here, we use the standard basis of the Ising interaction by exchanging σ_n^x and σ_n^z for convenience, but this simple change of basis does not

modify the essential physics in this system.
[9] G.-D. Lin et al., Europhys. Lett. 86, 60004 (2009).
[10] S. -L. Zhu, C. Monroe, and L. -M. Duan, Phys. Rev. Lett. **97**, 050505 (2006).
[11] H. T. Diep, Frustrated Spin System, World Scientific Publishing Company (2005).
[12] F. Barahona, J. Phys. A: Math. Gen. 15 3241 (982).
[13] Note that there is no phase transition in this region for even numbers of ions since the reflection symmetry is not spontaneously broken for even numbers of ions, which influences the phase stability.