Highly Degenerated Ground States in Some Rings Modeled by the Ising Spins with Competing Interactions

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We discuss three Ising ring systems with competing interactions which are analogs of quantum systems and we show that they exhibit similar properties. In particular, the archetypical system of three antiferromagnetically coupled spins \( s \) has two magnetically degenerated ground states with \( |M| = s \), when \( 0 < J_{ll} = \alpha < 1 = J_{12} = J_{23} \). The same effect is observed in the centered rings and even-numbered systems with antiferromagnetic couplings between the second neighbors which are the geometrically frustrated.

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1. Introduction

The notion of frustration in spin systems was introduced in the spin glass theory [1–3], but recently it has been studied in quantum spin systems, especially in the context of magnetic molecules built of transition metal ions with local spin \( s \) [4–12]. Kahn [15, 16] introduced a term “degenerate frustration” pointing out importance of the ground state (GS) degeneration in systems with competing interactions. On the other hand, studies of non-nuclear chromium molecules and their smaller analogues [5–10] not only have confirmed the Kahn results that the GS degeneration is present for a few well-determined values of a Hamiltonian parameter, but have shown that in a certain domain of this parameter the GS total spin \( S \) of geometrically frustrated spin system is the same as in the domain without the geometrical frustration. This specific region was assigned to the third type of frustration [5]. Some interesting results were obtained for quantum spin systems [9, 10]. For example, in the case of systems with one “defect” bond there is a series of 2s critical values of this coupling at which the GS degeneracy is present for a few well-determined values of \( \mu \) which lies in the domain without the geometric frustration. This specific region was assigned to the third type of frustration [5]. Some interesting results were obtained for quantum spin systems [9, 10].

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2. Rings with a bond defect

Energy of a configuration \( \mu \) is given as (\( n \) is an odd integer)

\[
E(\mu) = \sum_{j=1}^{n} m_{j} m_{j+1} + \alpha m_{1} m_{n}.
\]

For \( \alpha < 0 \) there is the unique GS \( \mu_{0} \) with \( m_{j} = (-1)^{j-1}s \) and energy \( E(\mu_{0}) = [(1 – n) + \alpha]s^{2} \) (Fig. 1a); in this state magnetization \( M(\mu) = \sum_{j=1}^{n} m_{j} = s \). When \( \alpha > 0 \) the system is geometrically frustrated and for large enough \( \alpha \) a pair of parallel spins has to be placed at one of the other \( n-1 \) bonds, so the degenerated GS contains, among others, \( n-1 \) “basic” configurations \( \mu_{j} \) with \( m_{j} = m_{j+1} \) for \( 1 \leq j < n \) and \( |M| = s \) (Fig. 1b). For \( s > \frac{1}{2} \) there are \( (n-2)(2s-1) \) “extra” GS’s \( \mu_{k,m} \), with \( m_{k} \), \( m_{k+1} \) and \( m_{k+2} < s \) (Fig. 1c). All these GS’s for \( \alpha > 1 \) yield geometric and energetic frustration, but with the non-degenerated GS are discussed below. Moreover, the GS’s are the same as those realized in non-frustrated systems, so the third type of frustration is revealed. A paradigm example is provided by antiferromagnetic rings with odd number of spin carriers (corresponding to the \( \text{Cr}_{n} \) molecule and its analogues). The second model describes antiferromagnetic rings with even number of spins uniformly coupled to an additional spin \( s_{0} \) related to Fe\(_{7}\) or Gd\(_{7}\) molecules [18, 19]. At the end rings with competing interactions of the first and the second neighbors are discussed.

The Heisenberg interactions \( s_{j} \cdot s_{k} \) are replaced by products of the \( z \)-components \( s_{j}^{z} s_{k}^{z} \) for arbitrary values of spin numbers \( s_{j} \). Energy of two coupled spins is \( E_{jk}(\mu) = J_{jk} m_{j} m_{k} \), where \( \mu = [m_{1}, \ldots, m_{n}] \), \( m_{j} \leq s \), \( 1 \leq j, k \leq n \), is the so-called Ising configuration. For \( \mathbf{F} = [-m_{1}, \ldots, -m_{n}] \) one has \( E_{jk}(\mathbf{F}) = -E_{jk}(\mu) \), then there is always trivial two-fold magnetic degeneration (except for all \( m_{j} = 0 \) which is neglected hereafter). Non-zero exchange integrals are antiferromagnetic with \( J_{jk} = -J_{kj} + \alpha \) for any real number \( \alpha \). Considered systems are homogeneous, so all \( s_{j} = s \).

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the GS energy $E(\mu_j) = E(\mu_{k,m}) - [(3 - n) - \alpha]s^2$. Both above discussed types of the GSC's are degenerated at $\alpha_c = 1$, $E = -(2n - n)s^2$, where $(2s - 1)$ additional states, with $|m_1| < s$ or $|m_n| < s$ have the same energy, so the total degeneration at $\alpha = 1$ equals $2ns$ (Fig. 1d).

3. Centered rings

For an even number $n$, spins $s_j$, 1 \leq j \leq n, are placed at vertexes of a regular polygon. They are coupled to the nearest neighbors, $J_{jj+1} = \alpha$, and uniformly to an extra spin $s_0$, $J_{0j} = \pm 1$, so $(n + 1 = 1)$

$$E(\mu) = \alpha \sum_{j=1}^{2n} m_j m_{j+1} + \varepsilon m_0 M_R, \quad M_R = \sum_{j=1}^{n} m_j, (2)$$

where $\varepsilon = \pm 1$; this system is geometrically frustrated for $\alpha > 0$. For $\alpha < 0$ the ring is ordered ferromagnetically, with $M_R = ns$, and $m_0 = -\varepsilon s$ (Fig. 2a). So, the GS energy equals $n(\alpha - 1)s^2$. For large values of $\alpha$ the first term dominates and the ring is ordered antiferromagnetically, $m_j = (-1)^{j-1}$ for 1 \leq j \leq n. Then $M_R = 0$ and the total energy, $-ns^2$, does not depend on $m_0$ and $\varepsilon$. So the degeneration of this GS equals $(2s + 1)$ (Fig. 2b). These two types of GS's are degenerated at $\alpha_c = 1/2$. Moreover, at this point many additional configurations enter the GS. Their number can be determined from combinatorial considerations, but this problem is left out in this paper. For $n = 4$ there are $8s(s + 1) - 2$ such configurations (Fig. 2c), so the total degeneration at $\alpha = 1/2$ amounts to $8s^2 + 10s$.

4. Second neighbors

Even-numbered rings become geometrically frustrated when antiferromagnetic interactions of the next-nearest neighbors are present. In the simplest, uniform case the energy is given as $(n + p = p)$

$$E(\mu) = \sum_{j=1}^{n} (m_j m_{j+1} + \alpha m_j m_{j+2}) . (3)$$

The second term describes two antiferromagnetic "subrings", which are geometrically frustrated when $n/2$ is an odd number. For $\alpha < 0$ the non-frustrated system has the unique antiferromagnetic GS with $E(\mu_{AF}) = n(\alpha - 1)s^2$ (Fig. 3a). Large $\alpha > 0$ should lead to antiferromagnetically ordered subrings. However, this is possible for $n/2$ even only, so the cases $n = 4q$ and $n = 4q + 2$ are discussed separately. In the first case, there are two non-equivalent antiferromagnetic configurations of subrings, so the two-fold degenerated GS comprises $\mu_{AF1} = [s, s, -s, -s, \ldots, -s, -s]$ and $\mu_{AF2} = [s, -s, -s, \ldots, -s, s]$ (Fig. 3b). Hence, the GS energy equals $E(\mu_{AF1,2}) = -ns^2$. Comparing this value with the previous result one obtains the critical value $\alpha_c = 1/2$. Additional states at $\alpha = 1/2$ enter the GS for $n > 4$ and, for example, there 20 such states (so 23 in total) for $n = 8$ and $s = 1/2$ (Fig. 3c). Note that presented configurations have $M = 0$ in the first two cases, whereas at $\alpha = 1/2$ some of them have $M \neq 0$.

For $n = 4q + 2$ (and large enough $\alpha > 0$), the subrings are geometrically frustrated and their configurations are degenerated, what increase the whole system GS degeneration in comparison with the previous case. The minimum energy amounts to $[(4n) - 2]s^2$ and the same
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ever, in each of these cases systems behave in different
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Fig. 4. Ground state configurations for the Ising-like

spins $s_j = 1$, $1 \leq j \leq 6$, placed at vertexes of a regular

hexagon ($J_{j+1} = 1$, $J_{j+2} = \alpha > 1/2$). Four typical

configurations are presented. Empty, black, and gray

circles denote $m_j = \pm 1$ and $m_j = 0$, respectively.

critical value $\alpha_{c,SN} - 1/2$ is obtained. For $\alpha > 1/2$ degen-

eration of the GS equals $n_0[\left(n - 4\right)n + 2]$ (Fig. 4). There

is no additional configurations at $\alpha = 1/2$ for $n = 6$, but
degeneration at this point increases rapidly for $n \geq 10$.

5. Summary

Three systems discussed above show some common fea-
tures. At first, the parameter $\alpha$ has the critical value

$\alpha_c > 0$, independent on the system size $n$ and the spin

number $s$. When $\alpha < \alpha_c$ the GS is not degenerated, ex-

cept for the trivial change $m_j \rightarrow -m_j$ for all spins $s_j$.

It has to be stressed that for $0 < \alpha < \alpha_c$ the systems

considered are geometrically (so also energetically) frus-
trated, but the degenerate (Kahn) frustration is absent.

Moreover, these systems retain appropriate GS’s from the

range $\alpha < 0$, where the geometrical frustration is absent.

In other words, despite the presence of competing inter-

actions ($J$ and $J'$, say) the systems considered do not

change their GS’s if the appropriate ratio $\alpha - |J' / J|$ is

small enough, i.e. $\alpha < \alpha_c$. Therefore, all of them exhibit

the third type of frustration in this domain. Analogous behavior has been found in the classical and quantum

counterparts of models discussed here [9, 10, 20]. How-

ever, in each of these cases systems behave in different

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what leads to two configurations with differ-
ent chirality). In the quantum systems the GS, which

is a linear combination of many Ising configurations $\mu$,

is modified in a continuous way except for a series of

well-determined “critical” values of $\alpha$, when the GS is

significantly changed. In both systems, the critical values

are size- and spin-dependent. The Ising-like model

shows the unique critical value with highly degenerated

GS when $\alpha \geq \alpha_c$.

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