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研究課題名（和文）Lattice and Charge Engineering of Spin Ice

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研究成果の概要（和文）：磁性物質の新奇な性質を理解し、制御することは現代物性物理学の主目的の一つである。磁性体はしばしば、原子間の相互作用のフラストレーションのために、微視的なレベルにおいて競合関係が生じる。数々の磁性体はこのようなフラストレーションの特性を持ち、結果として固有の興味深い特性が発現する。本プロジェクトでは従来の理論の扱いを越えて、フラストレーションの効果を考慮することにより、希土類磁性体の一群において、局所的な拘束条件に起因して生じる磁性複合体構造が引き起こす、興味深い非平衡現象を見出すことができた。我々の発見は磁性体において、トポロジカル欠陥を制御するための新しい指針を与えることが期待される。

研究成果の概要（英文）： One of the main motivation of modern research in Condensed Matter is to understand and control the unconventional properties of magnetic materials. Sometimes, the interaction between atoms is "frustrated", unable to accommodate all atoms at the same time, creating a competition at the microscopic level. An increasingly large variety of magnets appear to be "frustrated", each of them with their own exotic peculiarities. Our motivation in this project has been to go beyond the traditional theoretical models of magnetic frustration considering relevant, more complex, interactions. We have found, among other things, a surprisingly rich physics out of equilibrium in a family of rare-earth crystals, and low-temperature magnetic phases where microscopic local rules lead to extended fractal structures, opening new directions on how to control topological defects in magnets.

研究分野： 物性物理学理論

キーワード： frustrated magnetism　spin ice　spin liquid　topological defects

１．研究開始当初の背景

By preventing traditional ordering, magnetic frustration has opened a window for unexplored cooperative and topological phenomena in Condensed Matter. The spin-ice model is a canonical example of frustration with Ising spins, where topological defects take the form of magnetic monopoles. While this model is primarily applied to rare-earth pyrochlores in three dimensions, many of its properties are also shared by two-dimensional kagome systems.

２．研究の目的

Our motivation in this Kakenhi project has been to explore new directions of research related to spin ice, such as the search for new topological phases and the influence of itinerant electrons and lattice perturbations.

(A)
One of the remarkable recent discoveries in frustrated magnetism is the experimental observation of a “spontaneous” anomalous Hall effect (AHE) in the compound $Pr_2Ir_2O_7$ [1]. This phenomenon differs from traditional AHE in the sense that it has been measured in absence of any macroscopic magnetic moment. Because the apparition of the spontaneous AHE in $Pr_2Ir_2O_7$ is a probable consequence of out-of-equilibrium dynamics after a field quench in the [111] direction, our initial motivation has been to study a realistic minimal model able to support a variety of out-of-equilibrium phenomena after a similar field quench, without any persistent magnetisation. As discussed in the next “method” section, we introduced a corresponding spin model, and worked on this problem.

(B)
What happens when the spin model, which we have introduced in (A), is constrained within a plane ? This is what we have investigated on the kagome lattice [5], showing that it is also possible to map the corresponding Ising spin model onto an equivalent model of topological charges interacting at the nearest-neighbour level.

(C)
Pyrochlore and kagome antiferromagnets are archetypical examples of flat-band systems in frustrated magnetism. While these systems have been rather extensively studied, little is known about their “breathing” counterparts [6]. In breathing pyrochlores and kagomes, a broken symmetry of the lattice allows for the couplings between neighbouring frustrated units, namely the tetrahedra and the triangles respectively, to differ. Breathing lattices thus offer the possibility to explore a different facet of the rich physics of these systems, and have recently been synthesised in a series of materials on pyrochlores ($LiGaCr_4O_8$, $LiInCr_4O_8$, $Ba_3Yb_2Zn_5O_{11}$ …) and kagomes (vanadium oxyfluoride …)

３．研究の方法

(A)
The magnetic rare-earth ions of $Pr_2Ir_2O_7$ reside on the pyrochlore lattice and are to a first approximation Ising in nature, making the spin-ice model a good starting point. The influence of itinerant electrons in a Kondo lattice is often modelled by further neighbour interactions between the localised spins.

Using state-of-the-art Monte Carlo simulations, we have thus studied the spin-ice model, adding second J_2 and third J_3 neighbour interactions [2]. By fixing $J_2 = J_3 = J$, our spin model can be recast into a model of topological defects with nearest-neighbour coupling and a chemical potential for creation/annihilation of pairs of defects. This coupling can be chosen to be unconventional, or not, i.e. attractive or repulsive between defects.

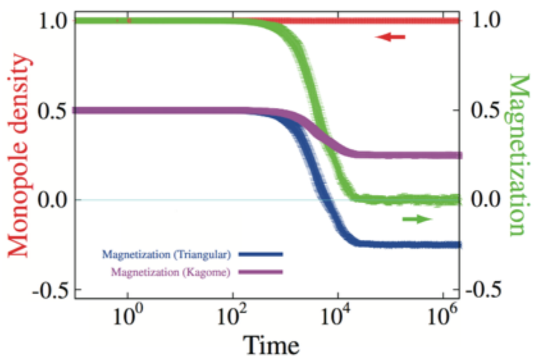
(B)
We have adopted the same spin-ice model as (A), defined on a kagome lattice, and studied this model, by combining classical Monte Carlo simulation and analytical Bethe approximation. In particular, we implemented a novel worm-algorithm to accelerate relaxation in the spin liquid region.

(C)
We have considered nearest-neighbour classical Heisenberg interactions, both ferromagnetic and antiferromagnetic, and studied how the anisotropy of breathing lattices modifies the mode spectrum of pyrochlore and kagome systems [7]. This work was analytical.

４．研究成果

(A)
For negative *J,* after a field quench, our model supports long-lived magnetisation

plateaux due to multi-scale energy barriers and subsequent dynamical bottlenecks [see Figure 1]. These magnetisation plateaux allow for the metastability of a “fragmented” spin liquid, an unconventional phase of matter where long-range order co-exists with a spin liquid, which has lately attracted the attention of the “frustrated-

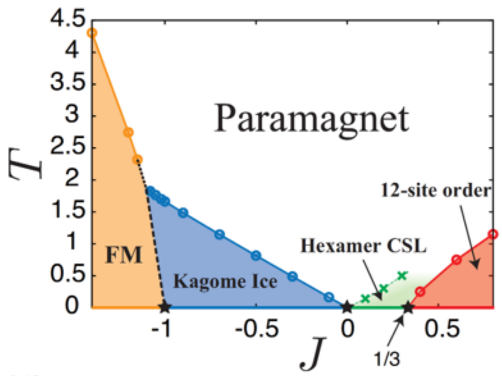


magnetism” community [3,4].

Figure 1: Time evolution of the monopole density and magnetization after a field quench. While the total magnetization ultimately vanishes (green curve), it gives rise to long-lived magnetization plateaux on pyrochlore layers perpendicular to the [111] direction (blue and violet). Noticeably, the magnetic relaxation occurs at constant monopole density (red). This long-lived regime corresponds to the metastable fragmented spin liquid where partial magnetic order co-exist with a Coulomb spin liquid.

For positive *J*, the attraction between same-sign charges produces clusters of these defects at equilibrium. The stability of these clusters is due to a combination of energy and topological barriers. These clusters may take the form of a “jellyfish” spin texture, centred on a closed ring with branches of arbitrary length. The ring carries a clockwise or counterclockwise circular flow of magnetisation. This emergent toroidal degrees of freedom provides a possibility for time-reversal symmetry breaking in absence of macroscopic magnetisation. Being inherently non-local and energetically stable, this toroidal degree of freedom can easily remain frozen over long time scale. Hence, in addition to a variety of out-of-equilibrium phenomena observed in a model without any quenched disorder (it is not a spin glass), and the discovery of stable extended magnetic textures made of topological defects, this emergent toroidal degrees of freedom offers a possible route of investigation for the spontaneous AHE in $Pr_2Ir_2O_7$.

(B)
Even for unconventional coupling between



the charges, i.e. where defects bearing the same charge attract each other, the system remains strongly constrained by the Gauss’ law. The resulting phase diagram supports a variety of (dis-)ordered phases, including what is, to the best of our knowledge, a yet unexplored classical spin liquid (CSL) [see Figure 2]. This CSL is made of clusters of same-sign charges, in a way reminiscent to the above pyrochlore model, but with the distinctive difference that the kagome lattice is entirely paved with such clusters; each cluster is surrounded by, and in direct contact with, clusters of opposite charges.

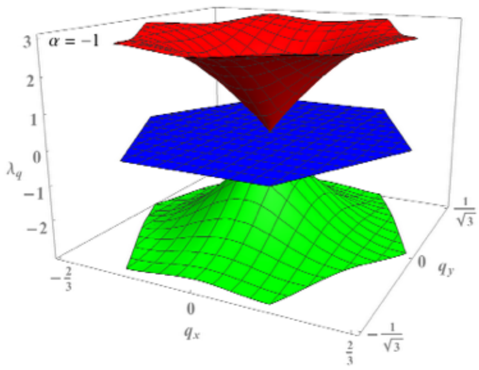
Figure 2: Phase diagram for attractive (*J<0*) and repulsive (*J>0*) interaction between charges of opposite sign with phase transitions (circles) and crossovers (crosses). There is no long-range order in the kexamer classical spin liquid (green).

This CSL is stable over an extended region of the phase diagram, and interestingly connected to the regime of small further neighbour coupling *J* [see Figure 2]. It is characterised by an extensive residual entropy of unconventional value, as well as the formation of hexamer rings of same-sign topological charges. The emergence of hexamers is reflected by a “half-moon” pattern in the magnetic structure factor, which provides a signature of this new spin liquid in neutron-scattering experiments.

This work opens the door for exciting new directions of research in the very active fields of two-dimensional spin liquids and interactions between fractionalized charges in Condensed Matter. Since this CSL phase is stable over an extended region of the phase diagram, the addition of quantum fluctuations would be especially interesting. As a side benefit, Monte Carlo simulations of this CSL have required the development of a worm algorithm which does not require the usual presence of a local conservation law, as opposed to traditional Coulomb spin liquids.

(C)
The nature and degeneracy of the flat bands are shown to be preserved for any value of the anisotropy. These flat bands can coexist with Dirac nodes at the Γ point when the model becomes particle-hole symmetric [see Figure 3].

Figure 3: Apparition of a Dirac cone in the



mode spectrum of the interaction matrix for breathing kagome when the model becomes particle-hole symmetric.

We have also derived the nature of the ground state for the breathing kagome lattice, both for the Heisenberg and XXZ Hamiltonians, which bears a spontaneous chirality when neighbouring triangles are alternatively ferro- and antiferro-magnetic.

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In conclusion, during this Kakenhi project, we have had the opportunity to study a palette of phenomena beyond the traditional frustrated spin-ice model:

(A)
complex out-of-equilibrium dynamics after a field quench in a system without quenched disorder, with possible connection to the AHE of $Pr_2Ir_2O_7$

(B)
new kinds of spin liquids made of clusters of topological charges: these clusters are diluted on pyrochlore, and fully packed on kagome

(C)
preservation of the flat bands in breathing lattices despite broken lattice symmetry, and apparition of Dirac cones in the mode spectrum of the interaction matrix

These results are very promising, and we have no doubt will nucleate further work in the topical fields of spin liquids, topological phases, flat-band systems, interactions between fractionalised charges and out-of-equilibrium dynamics away from traditional spin glasses.

If we may conclude on a more personal note, this Kakenhi project also corresponds to the time where both collaborators have moved on to Faculty positions: Masafumi Udagawa is Associate Professor in the University of Gakushuin since 2015, and Ludovic Jaubert is CNRS researcher in the University of Bordeaux in France since 2017

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2017年05月04日, Cambridge, UK
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(invited talk)

〔図書〕（計　0　件）

〔産業財産権〕

○出願状況（計　0　件）

名称：
発明者：
権利者：
種類：
番号：
出願年月日：
国内外の別：

○取得状況（計　0　件）

名称：
発明者：
権利者：
種類：
番号：
取得年月日：
国内外の別：

〔その他〕
ホームページ等
Personal webpages with publication list
https://www.loma.cnrs.fr/ludovic-jaubert/#tabpanel9
https://groups.oist.jp/tqm/publications

All papers were made freely available on arXiv:
https://arxiv.org/abs/1702.03794
https://arxiv.org/abs/1610.01748
https://arxiv.org/abs/1603.02872
https://arxiv.org/abs/1408.3669

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