

Magnetic order of non-magnetic ions

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Magnetism of a material originates from electrons in it since electrons behave as tiny magnets and align in the same direction in an ordinary macroscopic magnet. Such a property of an electron as a magnet is called spin. Thus, the basic researches for understanding and manipulating spins in materials are very important.

If there are two electrons in an ion, however, magnetism can be canceled out by aligning their spins in opposite directions. Such an ion is called a non-magnetic ion. We call an ion with an odd number of electrons a Kramers ion and an ion with an even number of electrons a non-Kramers ion. To become a non-magnetic ion, its spins need to be canceled out and it should be a non-Kramers ion. Conversely, a Kramers ion, for example, neodymium ion, is always a magnetic ion and a good candidate for an ingredient of a strong magnet.

On the other hand, non-magnetic ions cannot possess magnetism in an ordinary manner. However, surprisingly, according to quantum mechanics, which describes the microscopic world such as ion and electron, a magnetic object is possible to emerge from non-magnetic objects.

When we have two different non-magnetic states, by following a principle of quantum mechanics, it is allowed to construct a “superposed state” by adding these states with a coefficient of the imaginary unit i (Fig. 1). This state has circulating currents of the electrons and magnetism revives, since a circulating current generates a magnetic field like a electromagnet. In this state, the magnetic field produced by the currents cannot be described as a single magnet, since the direction of the axis of the circulation changes depending on position. Such a state is described by a complex of magnets and is called a higher-order magnetic state.

Such higher-order magnetic states have been investigated and actually discovered in some materials [1-3], but only in materials with magnetic ions to date.

To investigate whether it is possible to realize such a magnetic state from non-magnetic states, we have studied a theoretical model for non-Kramers ions with two electrons in each ion [4]. In this model, we can compose two non-magnetic states for each ion with different shape of electron distribution as shown in Fig. 1. In both states, the spins of the two electrons align opposite directions and magnetism is canceled out. Then, we search for stable states for several kinds of lattice structure. We find that the alignment of the non-magnetic states [non-magnetic order, Fig. 2(a)] occurs when ions align along a direction of a lattice axis. On the other hand, the alignment of the magnetic states [magnetic order, Fig. 2(b)] occurs when ions align along a diagonal direction. Thus, it is interesting to search lattices in which ions locate diagonal directions for such an exotic magnetic state.

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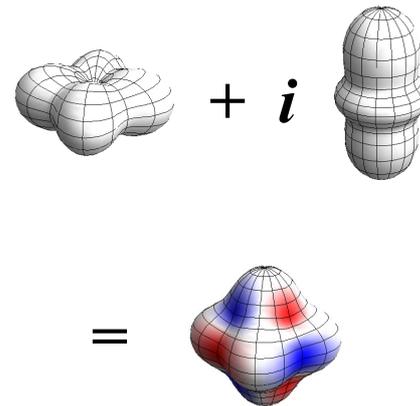


Fig. 1 Magnetic state composed of non-magnetic states with different shape of electron distribution. In the red and blue areas, the axes of the circulating currents are in opposite directions and produce opposite magnetic fields.

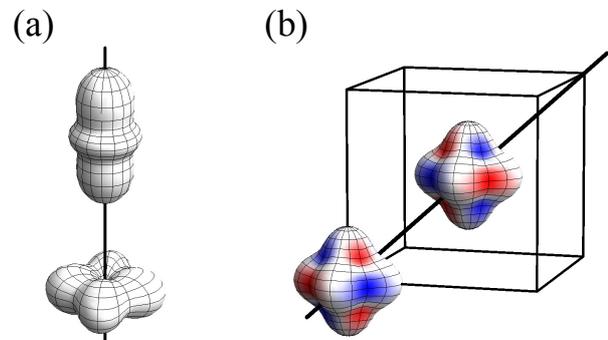


Fig. 2 (a) Non-magnetic state for ions aligned along a direction of a lattice axis. (b) Magnetic state for ions aligned along a diagonal direction.

Reference

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- [4] [K. Kubo *et al.*, Phys. Rev. B **95**, 054425 \(2017\).](#)