Mapping of theoretical approach in magnetics

– coarse graining theory–

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Nowadays, the objects for magnetics are spreading to various fields. Under those circumstance, the requirements to theoretical analysis increase, i.e. a simple modeling, numerical prediction, etc. Besides, the requests such as materials predictions based on the data base analysis called “materials informatics” or “material genome” become strong, too.

Generally, from a viewpoint of magnetics, it is necessary to understand the magnetization distribution and/or a magnetization process in devices and materials. In this sense, the micromagnetics theory is convenient to understand the side view of the phenomenalism. However, that theory is insufficient to define the exact property, because it does not include self-consistency of theory. To obtain the accurate magnetic property, the knowledge from a microscopic theory should be required.

For the discussion of magnetization state, the magnetic energy can be defined by following procedure,

1) Spin–spin interaction (including the exchange interaction, spin transfer) is evaluated within a framework of electric theory.
2) The magnetic anisotropy constant is evaluated within a framework of first principles calculation for certain materials.
3) The magnetic dipole interaction is generally evaluated by the numerical calculation of a classical spin model.
4) The thermo-dynamic behavior of magnetization is evaluated by the statistical average of a classical spin model.

Then, the obtained magnetic energies reflect onto the micromagnetics calculation. At this point, the atomistic calculation is ready to carry out.

However, to analyze the entire body of materials and devices, the atomistic calculation needs to expend too much computational resources. In this sense, it is required well defined coarse graining theory for connecting atomistic calculations and conventional micromagnetics calculations.

In terms of energy evaluation 3), the multipole expansion method naturally deals with the magnetic dipole interaction, in which the contribution from the distant part is averaged over a certain volume. For 4), the formulation of the Landau-Lifshitz-Bloch equation is suggested[1)], which includes the degree of freedom for permitting the expansion and

contraction of the magnetization vector. For 1), the method of single spin approximation[2)] is one of the candidate to deal with the exchange interaction between the textured grains. Finally, for 2), the conversion from a single site anisotropy to the expression of energy density form simply satisfies the coarse graining.

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Fundamental knowledge of first-principles calculation

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In this tutorial talk, the fundamentals of first-principles calculation are briefly reviewed for beginners. The theoretical framework of first-principles calculation, i.e. so-called density-functional theory was established by Hohenberg and Kohn[1]. They probed that the ground-state energy of an inhomogeneous electron gas can be expressed as a functional of the electron density $n(\boldsymbol{r})$ and the energy functional takes its minimum value for the correct ground-state. The advantage of the theory is that we need no explicit expression for the wave function of an interacting electron system. The density-functional theory gives us a firm base for understanding the complex interacting electron systems. However, no one knows an explicit expression of the energy functional. A practical method treating an interacting electron system was proposed by Kohn and Sham[2] on the basis of the density-functional theory. They reduced the many-body problem of interacting electron systems to self-consistent equations, i.e. Kohn-Sham equations, for single electron in an effective potential, which contains exchange and correlation terms. They assumed that the exchange and correlation potentials depend only on the electron density at the position where the potential is acting. We usually adopt the explicit form of the exchange and correlation potentials for a homogeneous electron gas. This is called local density approximation (LDA). The treatment enables us to obtain the ground state energy as well as the energy band-structure of complex systems such as molecules and solids. However, there are drawbacks originated from the LDA; overestimation of cohesive energy and hence underestimation of inter-atomic distances, underestimation of band gap of semiconductors or insulators including Mott-Hubbard insulators caused by electron correlation effect, underestimation of exchange splitting of spin-up and down bands in magnetic materials, and so on. Some of these drawbacks can be overcome by improved treatments of the exchange and correlation potentials; i.e. generalized gradient approximation[3], self-interaction correction[4], LDA+U method[5], self-energy correction including GW approximation[6] and dynamical mean-field approximation[7], and so on. Typical examples calculated with use of these approaches are presented and the shortcoming of them will be discussed.

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磁化構造中の伝導電子の理論

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Theory of electron transport in the presence of magnetization textures

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1　Introduction

In this paper, we discuss two topics, an emergent electromagnetic field which couples to electron's spin in ferromagnetic metals [1] and current-induced torques [2] from the theoretical viewpoints.

Our technology is based on various electromagnetic phenomena. For designing electronics devices, thus, the Maxwell's equation is of essential importance. The mathematical structure of the electromagnetic field is governed by a U(1) gauge symmetry, i.e., an invariance of physical laws under phase transformations. The gauge symmetry is equivalent to the conservation of the electric charge, and was established when a symmetry breaking of unified force occured immediately after the big bang. The beautiful mathematical structure of charge electromagnetism was therefore determined when our universe started, and there is no way to modify its laws.

Fortunately, charge electromagnetism is not the only electromagnetism allowed in the nature. In fact, electromagnetism arises whenever there is a U(1) gauge symmetry associated with conservation of some effective charge. In solids, there are several systems which have the U(1) gauge symmetry as a good approximation. Solids could thus display several types of effective electromagnetic fields. A typical example is a ferromagnetic metal. In ferromagnetic metals, conduction electron spin (mostly s electron) is coupled to the magnetization (or localized spins of d electrons) by an interaction called the sd interaction, which tends to align the electron spin parallel (or anti-parallel) to the localized spin. This interaction is strong in most $3d$ ferromagnetic metals, and as a result, conduction electron's spin originally consisting of three components, reduces to a single component along the localized spin direction. The remaining component is invariant under a phase transformation, i.e., has a U(1) gauge symmetry just like the electric charge does. A spin electromagnetic field thus emerges that couples to conduction electron's spin. The first subject of the present paper is this spin electromagnetic field. The world of spin electromagnetic field is richer than that of electric charge, since the electron's spin in solids is under influence of various interactions such as spin-orbit interaction. We will in fact show that magnetic monopole emerges from spin relaxation processes. Spin electromagnetic field drives electron's spin, and thus plays an essential role in spintronics. The other subject, the current-induced torques, is a reciprocal effect of spin electromagnetic field.

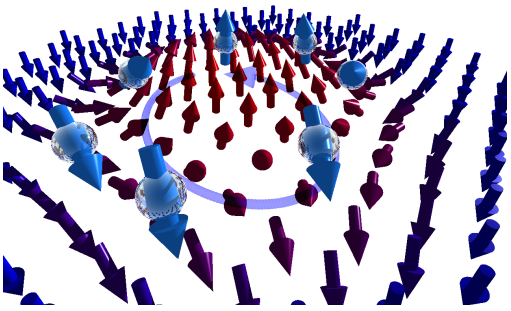

Fig. 1　The spin of a conduction electron is rotated by a strong sd interaction with magnetization as it moves in the presence of a magnetization texture, resulting in a Berry's phase factor $e^{i\varphi}$

The effect of spin electromagnetic field was partially discussed already in 1986 by Berger, who discussed a voltage generated by a canting of wall plane of a driven domain wall [3]. Emergence of effective electromagnetism coupling to electron's spin was pointed out by use of gauge field argument by Volovik in 1987 (Ref. [4]). Stern discussed the motive force in the context of the spin Berry's phase, and discussed similarity to the Faraday's law [5]. Spin motive force was rederived in Ref. [6] in the case of domain wall motion. It was argued in the context of topological pumping in Ref. [7]. Duine discussed spin electric field including the effect of spin relaxation by use of non-adiabaticity parameter (β) [8,9]. The Hall current induced by a spin electric field in the presence of spin-orbit interaction was theoretically studied by Shibata and Kohno [10,11]. The effect of Rashba

interaction on spin electric field was discussed in Refs. [12,13]. These works [6,8,10,12,13] have focused solely on the spin electric field. The magnetic component of Rashba-induced spin electromagnetic was discussed in Ref. [14].

2 Emergence of spin gauge field

Let us here demonstrate that a spin gauge field emerges from a strong *sd* exchange interaction (adiabatic limit). Because of the *sd* interaction, spin of electron traveling through a magnetization structure follows the local spin and rotates with it (Fig. 1), and the spin acquires a geometric phase [15]. The phase is written as an integral of an effective gauge field, $\boldsymbol{A}_{\rm s}$, along its path C as $\varphi = \frac{e}{\hbar}\int_C d\boldsymbol{r}\cdot\boldsymbol{A}_{\rm s}$, where e is electron charge and $\hbar$ is the Planck's constant devided by 2π. The vector $\boldsymbol{A}_{\rm s}$ turns out to be

$$\boldsymbol{A}_{\rm s} = \frac{\hbar}{2e}(1-\cos\theta)\nabla\phi. \tag{1}$$

Existence of the phase means that there is an effective magnetic field, $\boldsymbol{B}_{\rm s}$, as seen by rewriting the integral over a closed path using the Stokes theorem $\varphi = \frac{e}{\hbar}\int_S d\boldsymbol{S}\cdot\boldsymbol{B}_{\rm s}$, where $\boldsymbol{B}_{\rm s} \equiv \nabla\times\boldsymbol{A}_{\rm s}$ represents curvature. This phase φ attached to electron spin is called the spin Berry's phase. Time-derivative of phase is equivalent to a voltage, and thus we have effective electric field defined by $\dot{\varphi} = -\frac{e}{\hbar}\int_C d\boldsymbol{r}\cdot\boldsymbol{E}_{\rm s}$, where $\boldsymbol{E}_{\rm s} \equiv -\dot{\boldsymbol{A}}_{\rm s}$. $\boldsymbol{E}_{\rm s}$ and $\boldsymbol{B}_{\rm s}$ are called spin electric and magnetic field, respectively. They satisfy the Faraday's law,

$$\nabla\times\boldsymbol{E}_{\rm s} + \dot{\boldsymbol{B}}_{\rm s} = 0, \tag{2}$$

as a trivial result of their definitions. The fields have a structure of electromagnetism and thus a spin electromagnetic field coupled to electron's spin emerges. One should note that those fields are real or observable ones coupling to real electric charge and current and not just 'fictitious fields'.

In the presentation, phenomena arising from the spin gauge field, Eq. (1), are discussed.

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Numerical methods for quantum magnets

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Methods for studies on quantum magnets are overviewed. In the classical picture, spin can be regarded as a vector of magnetic moment. But, various interesting properties due to the quantum effects have been studied as the so-called 'quantum spin systems'[1]. Quantum mechanical effect in spin systems is originated in the non-commutative property of spin operators: $[S_x, S_y] = i\hbar S_z$, etc. In order to take into account the quantum effect, we need to treat the Hamiltonian matrix $\mathcal{H}$ of the system whose matrix is of 2^Nx2^N for a system consisting of N spins of S=1/2. The straightest way to study the system is a diagonalization method to obtain the eigenvalues and eigenvectors of the matrix. To study finite temperature properties, we calculate Tr exp(-β$\mathcal{H}$), and we need all the eigenvalues and eigenvectors[2]. However, often we are interested in low temperature properties of the system, in particular the ground system. There, we may use iterative methods for the low energy states, such as the Lanczos method. For such purpose, TIT-pack was released[3], which encouraged studies in this field in Japan, and several method to extrapolate the data has been developed.[4]. But, the system size is still limited.

To study a large system a quantum Monte Carlo (QMC) method by making use of the Suzuki-Trotter method[5] has been introduced. This method has been developed with the idea of the loop algorithm and the continuous imaginary time algorithm[6], and methods to take into account effects of lattice distortion have been also developed. Now QMC is the one of the most reliable methods for quantum many body systems. However, the method consists of a sampling of the so called world lines (paths in the path-integral method) [7], and suffers from the so-called 'negative sign' problem, and cannot be applied to frustrated system efficiently.

As an efficient method to study large systems in one dimension (1D), the so-called DMRG (density matrix renormalization group) method was invented[8]. The idea of this method has been developed and is now one of the most powerful method for 1D systems. This method is extended to higher dimensions[9] also to finite temperatures. The similar idea has been introduced as the matrix-product method[10], and recently it has been studied extensively as tensor-network methods.[11]

Magnetic resonance is also an important subject of the study of magnetism. The ESR spectrum is given by Kubo formula. As a microscopic approach, a direct calculation of the formula by making use of full diagonalization has been introduced[12], which gives precise information of the spectrum for given systems, e.g., the effect of spatial configuration of the lattice, the dependence on the field direction. Application of this method is also limited to small sizes because it uses diagonalization of the system Hamiltonian. For the ESR spectrum in the ground state, we may use the idea of Lanczos method, and also DMRG (dynamical DMRG)[13,14]. For finite temperatures we can make use of the time evolution of the so-called typical state.[15,16,17] The field and temperature dependent in 1D systems has been studied bay making use of field theoretical informations[18]. The typical state would give a seminal method to give temperature dependent thermal properties[17].

Moreover quantum dynamics is also an important issue in quantum magnets. The dynamics of magnetization under time dependent field reflects the energy level structure of the system. Such effect was observed in single molecular magnets (SMM) such as Mn12, Fe8, and V15, etc. [19] The importance of the Landau-Zener process was pointed out.[20] The dynamics in dissipative environments is treated by the quantum master equation[21]. The combination of quantum dynamics and dissipative effects provides interesting phenomena, such as the phonon-bottleneck effect or magnetic Foehn effect[22]. Recently the hybridization between magnetic state and photon state in a cavity attracts interests in the context of manipulation of quantum state. The quantum master equation is also used to emulate such quantum dynamics[23]. In quantum systems, the so-called quantum fluctuation plays an important role. By making this fact, the so-called quantum annealing method was invented[24]. This method is used in a quantum computing of the D-wave machine.[25]

With the development of super-computer such as the K-computer, massive parallel algorithm allows us to use a large

memory. Such technique has been established, and now systems with more than 40 spins (S=1/2), can be calculated.[26] Recently the system ALPS is released for non-specialists, in which some of the above methods are prepared in user-friendly way[27].

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Micromagnetic Simulation

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Since the pioneering works by Brown and LaBonte[1-3], micromagnetic simulation has been used to calculate the magnetization distribution and its dynamics in nanoscale magnetic materials. Because of the limitations of the calculation speed of the computers, they proposed the simple algorithms to obtain the energy minimum state, and solved the problem within these limitations[1-6]. Usually, the exchange, anisotropy, Zeeman, and the demagnetizing energies are considered in micromagnetic simulation.

$$\varepsilon = A(\nabla \mathbf{m})^2 + K_u \sin^2\theta - \frac{1}{2}\mathbf{H}^D \cdot \mathbf{m} - \mathbf{H}^E \cdot \mathbf{m}. \qquad (1)$$

Here, A, K_u, $\boldsymbol{H^D}$ and $\boldsymbol{H^E}$ are the exchange stiffness constant, the uniaxial anisotropy constant, the demagnetizing field and the external field, respectively.

In 1980s, third generation supercomputers appeared and they extended the limitations. Micromagnetic simulation was used to solve some problems, i.e., the magnetic domain wall dynamics[7,8], magnetic fine particle[9,10], magnetic thin film[11], magnetic recording media[12], and magneto-optical recording media[13]. In these reports, Landau-Lifshitz-Gilbert equation was used.

$$\dot{\mathbf{m}} = -\gamma \mathbf{m} \times \mathbf{H} - \frac{\alpha}{M_s}\dot{\mathbf{m}} \times \mathbf{m}. \qquad (2)$$

$$\rightarrow \dot{\mathbf{m}} = -\frac{\gamma}{1+\alpha^2}\left[\mathbf{m} \times \mathbf{H} + \alpha\left[\mathbf{m} \times (\mathbf{m} \times \mathbf{H})\right]\right]. \qquad (3)$$

$$\mathbf{H} = -\frac{\delta \varepsilon}{\delta \mathbf{m}}. \qquad (4)$$

Here $\boldsymbol{H}$ is the effective field acting on the magnetic moments. It is calculated by using eq. (4). However since the calculations of the demagnetizing field required a lot of calculation time even with the supercomputers[14,15], they could not solve the LLG equation with original form in many cases. However in these cases, they only needed the switching field of magnetic fine particles or thin films, and did not need the dynamics of the magnetic moments. In the cases, they dropped the gyroscopic term from the LLG equation (eq.(5)), and used a unity of the Gilbert damping constant to reduce the calculation time [9-12].

$$\dot{\mathbf{m}} = -\frac{\gamma}{1+\alpha^2}\left[\alpha\left[\mathbf{m} \times (\mathbf{m} \times \mathbf{H})\right]\right] \qquad (5)$$

In 1990s, the fast Fourier transform (FFT) algorithms were introduced to calculate the demagnetizing field[19,20]. It reduced the calculation time drastically. By using this algorithm, the LLG equation with original form can be solved, and larger scale and longer time simulation can be done with personal computers. Nowadays, there are many open source programs and products for micromagnetic simulation[21], micromagnetic simulation is used in many fields, such as nanospintronics, permanent magnet, etc, not only to analyze the experimental results, but also to obtain the optimum conditions of nanodevices. Recently, many effects except for in eq. (1) are discussing, such as Rashba field effect, spin hall effect, Dzyaloshinsky-Moriya interaction, etc. These effects can be adapted to the simulation as the effective field. However even with the personal computers in recent years, the size of the simulation region, which can be simulated within the acceptable time, is about ～0.5 μ m^2 in 2D model case. For larger scale or long time simulations, special computers such as GPU or massively parallel computers are required[22].

For the experimentalist, one of the interested points for the simulation is comparison of the simulation and experimental results. In case of the simple structure target, such as a single crystal material, simulation results in good agreement with the experimental results without special modification of the simulation model. However in case of the complex structure target, such as polycrystalline material, many modifications of the simulation model are required. In the presentation, the simulation results in these two cases will be presented[23-24]. The important points for the simulation will be also presented.

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Finite Element Analysis for Electromechanical Design

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Finite Element Analysis (FEA) is indispensable to design and development of electromagnetic field applications in industry as well as academic and several software packages for FEA are commercially available today. The basics of ElectroMagnetic (EM) FEA, use cases and future work will be explained here. It should be noted that electromagnetic applications can be classified into two categories, i.e. High Frequency (HF) and Low Frequency (LF) and this explanation will focus on the LF. Although the names imply that there exists a frequency as the divider, no such a clear boundary frequency exists since the divider is significance of the displacement current in the application's phenomena. Typical applications of HF are antennas, microstriplines and waveguides. LF, on the other hand, has motors, transformers and sensors, in which the magnetic field is dominant over the electric field.

The EM FEA was started in late of 1970 in the electrical engineering by utilizing the structural FEA technology which was originally developed for computational vibration analysis for aircraft in late 1960[1)]. The applications in the early stage were power transformers and generators[2)] for both of which prototyping is difficult due to the size and sophisticated design is required to achieve high efficiency and reliability for power supply in social infrastructure. Those successes expanded its application range to other systems and products such as TV tubes[3)4)], solenoid valves[5)], magnetic recording heads[6)], EM shields[7)], induction heating systems[8)], non-destructive testing[9)]. In the mid of 1990, as well known as Kyoto Protocol, the energy efficiency improvement became a must time in most electrical applications such air-conditioners[10)] and electric vehicles (EV)[11)] and hybrid vehicles (HV)[12)13)] which have to have very high efficient motors. To achieve the super high efficiency, the FEA was heavily used and it is still going on today.

The basic equation of the EM FEA is the Maxwell's equations with two constitutive equations which represent material characteristics and the displacement current term is omitted from them for LF. This modification decouples electric field from magnetic field so that it becomes easier to solve three equations rather than all the four equations. The drawback is, of course, one cannot see electric field effects such as displacement current flowing in a capacitor.

It does not mean LF is easier than HF in which one has to solve the four equations because, in LF, there exists magnetic saturation that leads to the non-linear problem and many applications have motion which is difficult to handle for EM where both space and objects are have to be modeled.

The remaining three equations can be unified by introducing magnetic vector potential instead of handling magnetic field directly.

The unified equation is transformed by Finite Element Method (FEM) into a form which can be solved by computers. In FEM, an analysis region, which includes magnetic materials, conductors and spaces, and time are discretized into small elements and time intervals. The union of elements is called mesh. The field value, which is magnetic vector potential in this case, is represented with a polynomial using interpolation functions. It means that the accuracy of the solution depends on the discretization, that is that smaller elements and time interval will give more accuracy.

The resulting discretized equation forms a matrix equation in which the coefficient matrix contains material characteristics and the load vector contains currents/voltage/permanent magnet. It is solved by a linear equation solver to obtain the magnetic vector potential. Recalling that the magnetic materials usually have complex behavior such as magnetic saturation and hysteresis characteristics, the equation is basically non-linear and needs to be solved with iterative manner. It should be noted that the dimension of the matrix increases as the number of the elements increases so that efficient meshing techniques is important to generate efficient meshes which have enough elements only for sensitive regions minimizing the total number of elements. After obtaining the magnetic vector potential, several physical quantities are naturally derived, such as magnetic flux density, magnetization, eddy current, losses, force and torque.

Today's challenges in the EM FEA are material modeling and high speed calculation for large scale models. Since material characteristics are basically given parameters for the equation[14)], the accuracy of the characteristics will directly affect the accuracy of the solution. On the other hand, behavior of material is so complex[15)] that it is difficult to have a material model which reproduces the behavior with reasonable costs. Although it is, of course, possible to use

the micro magnetic simulation techniques such as the material model, there are two significant problems which are enormous calculation cost and the fact that it is difficult to obtain parameters for the model by usual material measurements. Eventually, relatively simple material models, which is costless and can be constructed with measurable parameters, are employed in today's practical situations accepting certain inaccuracy. In this context, several new material models have been proposed and being examined.
The high speed calculation is natural sequence of pursuing highly accurate solution which is required for today's sophisticated detail design in advanced applications such as EV/HV. The main stream of speeding up is utilizing multi-/many cores equipped in the latest computing systems, that is parallel computing. However, the calculation scheme of EM FEM is not easily parallelized by its nature and many new ideas are required.
The EM FEA is actively used for wide range of applications and is still attracting users because of its powerful and flexible functionality. The technical challenges are going on to enhance the functionality and it is still evolving.

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