

論文 / 著書情報  
Article / Book Information

題目(和文)	フォノン角運動量の生成と変換の理論
Title(English)	Theory of Generation and Conversion of Phonon Angular Momentum
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出典(和文)	学位:博士(理学), 学位授与機関:東京工業大学, 報告番号:甲第11043号, 授与年月日:2019年3月26日, 学位の種別:課程博士, 審査員:村上 修一,齋藤 晋,笹本 智弘,吉野 淳二,西田 祐介
Citation(English)	Degree:Doctor (Science), Conferring organization: Tokyo Institute of Technology, Report number:甲第11043号, Conferred date:2019/3/26, Degree Type:Course doctor, Examiner:,,,,,
学位種別(和文)	博士論文
Category(English)	Doctoral Thesis
種別(和文)	要約
Type(English)	Outline

# Theory of Generation and Conversion of Phonon Angular Momentum

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February 2019

# Chapter 1

## Introduction

### 1.1 Introduction

Various excitations in solids have been among the most important subjects in solid state physics, because they exhibit various novel properties in a variety of materials. Representative examples are electrons, photons, phonons, and magnons. In quantum theory, light and electromagnetic waves have both wave nature and particle nature, and it is called photon. Similarly, the lattice vibration of each atom in crystals and the propagating waves have both particle and wave natures, and it is called phonon. Here, phonons represent collective vibrations, and they are not real particles. Unlike photons, phonons are classified into longitudinal and transverse waves. Phonons are classified into acoustic modes, where the neighboring atoms vibrate in the same phases, and optical modes, where the neighboring atoms vibrate in opposite phase, when there are two or more atoms in a unit cell. Phonons have been studied for a long time. Since phonons carry heat in solids, thermal conductivity and specific heat are closely related to a phonon dispersion in solids. It is also known that phonons interact with other elementary excitations. As an example of the interaction between electrons and phonons, in the jellium model, consisting of free electrons and uniform distribution of positive ions, a compression wave of a positive charge is generated by compression of waves in the longitudinal phonons. Then, the resulting periodic electric field having the same period with phonons combines with free electrons and attenuates sound waves. As another example, the electron-phonon interaction in a metal causes an effective attractive force between electrons, and it gives rise to superconductivity. For the interaction between photons and phonons, when a monochromatic light  $\omega_0$  is injected into a solid, the photoelectric field produces the dipole moment in the solids  $\mu = \alpha E_0 \cos \omega_0 t$  with the polarizability tensor  $\alpha$ . The phonons slightly alter the polarizability tensor at the phonon frequency  $\omega$ . Then, the dipole moment is

modulated and has a vibration component of  $\omega_0 \pm \omega$ , and the light emitted therefrom has the same vibration component. This scattering phenomenon is called Raman scattering. As described above, interaction of phonons with other elementary excitations have been intensively studied.

In recent years, the control of phonon degree of freedom has been an active field for experimental and theoretical studies. Phononics is a new active field aiming at controlling phonon dynamics and information transport by phonons. One of the recent topics in phononics is the phonon Hall effect [1, 2, 3, 4, 5, 6, 7, 8, 9]. Apart from phonons, the Hall effect of the electrons system has been known for a long time. When a magnetic field is applied perpendicular to the electric current, the electromotive force appears in a direction orthogonal to both the electric current and the magnetic field due to the Lorentz force. In the phonon Hall effect, when a heat current is used instead of a electric current, a temperature gradient occurs in a direction perpendicular to both the heat current and the magnetic field. This phenomenon was experimentally observed in ionic paramagnetic dielectrics, such as  $\text{Ta}_3\text{Ga}_5\text{O}_{12}$ (TGG) [1, 2], and in a quantum spin liquid candidate  $\text{Ba}_3\text{CuSb}_2\text{O}_9$  [3]. What is surprising is that, unlike electrons, phonons are quasi-particles without both charges and spins, and it cannot be directly coupled via Lorentz force. In one of the theoretical interpretations [6, 7], it is attributed to the spin-phonon interaction [10, 11, 12, 13, 14] which is the coupling between localized spin and lattice vibration. However, the experimental result and the theory is not consistent, and the fundamental mechanism is still not clear. Furthermore, new properties of phonons are proposed, leading to novel topological phenomena, analogous to quantum (anomalous) Hall effect and a topological insulator in electronics systems. The quantum (anomalous) Hall effect is characterized by a topological invariant called the Chern number of the first class, which is defined by an integral of the Berry curvature over the Brillouin zone and can be nonzero only for systems with broken time-reversal symmetry. The phononic states with nonzero Chern number give the quantum (anomalous) Hall-like edge states of phonons, which are topologically protected to be gapless, one-way, and immune to backscattering. Moreover, one of the merit in phononics systems is topological modes can be realized in macroscopic systems, such as the mechanical honeycomb lattice [15, 16, 17, 18, 19, 20], which is formed by the spring and mass, and the sonic crystal [21, 22], which consists of triangular polymethyl methacrylate rods positioned in a triangular lattice. For example, it was theoretically proposed that the Chern number has nonzero values in the phonon system where the time-reversal symmetry is broken by a mechanical rotation [20].

With the discovery of the phonon Hall effect, the angular momentum of phonon was proposed [23, 24, 25]. Unlike the general macroscopic rigid-body rotation, the phonon angular momentum is understood as microscopic local rotations of the atoms around their equilibrium positions in crystals. By extending this idea, the

concept of chiral phonon [26], namely, the phonon with phonon angular momentum was theoretically proposed. Subsequently, the chiral phonon is observed in tungsten diselenide [27].

## 1.2 Purpose of this thesis

In this thesis, we focus on how to generate this phonon angular momentum and to convert it to other degree of freedom. We focus on the conversion between the electron spin and the mechanical rotation. In magnetics, the Einstein-de Haas effect [28] and the Barnett effect [29] are known to convert between a magnetization and mechanical rotation. In the Einstein-de Haas effect when a magnetic material is magnetized by the external magnetic field, the magnetic material rotates around the external magnetic field to conserve the total angular momentum. The Barnett effect is a reciprocal effect to the Einstein-de Haas effect. The origin of spin conversion in these effect is considered to be the spin-rotation coupling [30, 31, 32, 33] which couples spin and mechanical rotation. Moreover, in spintronics, a method to generate a spin current via spin-rotation coupling has been reported theoretically and experimentally, such as a surface acoustic wave [34, 35], the twisting vibrational mode in a carbon nanotube [36], and the flow of a liquid metal [37]. In this way, the conversion between a spin and a mechanical rotation has been studied intensively. We focus on the phonon angular momentum. Our first purpose is to investigate the microscopic mechanism of the conversion between the electron spin and the microscopic local rotation. We also form on generation of phonon angular momentum, because the generation of phonon angular momentum is not well-known. Our second purpose is to clarify how to generate the phonon angular momentum and observation method. In the system without the inversion (time-reversal) symmetry, the phonon angular momentum of each phonon mode is an odd (even) function of wave vectors. In order to make the phonon angular momentum nonzero, the time-reversal or the inversion symmetries should be broken. In previous study [23], in the system without the time-reversal symmetry, such as the system under a magnetic field, the total phonon angular momentum have a finite value in equilibrium. On the other hand, in the system without the inversion symmetry, the total phonon angular momentum vanish because the phonon angular momentum of each phonon mode cancels between wave vectors  $\mathbf{k}$  and  $-\mathbf{k}$ . In this thesis, we propose a new method to generate the phonon angular momentum in systems without the inversion symmetry. Moreover, since the phonon angular momentum cannot be directly observed, we propose conversion of the phonon angular momentum to other degree of freedom.

## 1.3 Organization of this thesis

In this thesis, we discuss generation of the phonon angular momentum in non-magnetic crystals and magnetic crystals, and we propose experimental observation methods of the phonon angular momentum. Moreover, we discuss the spin magnetization due to the microscopic local rotation using a simple toy model. In chapter 2, we introduce the background of the present work: the overview of the lattice dynamics and the phonon, the review of the phonon angular momentum, and the overview of cross-correlated response and symmetry. In chapter 3, 4, and 5, we develop our study. In chapter 3, we discuss the generation of the phonon angular momentum by temperature gradient in the non-magnetic crystals without inversion symmetry. We also show numerical results of the phonon angular momentum generated by temperature gradient in the wurtzite GaN, Te, and Se. Moreover, we propose experimental observation methods of the phonon angular momentum, such as the conversions to a rigid-body rotation in solids and to a magnetization. In chapter 4, we discuss phonon angular momentum in the magnetic crystals without both the time-reversal and the inversion symmetries. We show the phonon angular momentum generated by the electric field in our toy model. In chapter 5, we discuss the microscopic mechanism of the conversion between the electron spin and the microscopic local rotation. We show that the electron spin expectation value along the microscopic rotational axis is proportional to the angular velocity of the microscopic local rotation in the adiabatic approximation. In chapter 6, we summarize this thesis.

# Publication List

Chapter 3 partially includes contents in the following publications:

1. Masato Hamada, Takehito Yokoyama, and Shuichi Murakami, “Spin current generation and magnetic response in carbon nanotubes by the twisting phonon mode”, Phys. Rev. B **92**, 060409 (2015).  
DOI:<https://doi.org/10.1103/PhysRevB.92.060409>  
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2. Masato Hamada, Emi Minamitani, Motoaki Hirayama, and Shuichi Murakami, “Phonon Angular Momentum Induced by the Temperature Gradient”, Phys. Rev. Lett. **121**, 175301 (2018).  
DOI:<https://doi.org/10.1103/PhysRevLett.121.175301>  
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