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Theory of electric polarization and spin magnetization in inhomogeneous crystals

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Abstract

Electromagnetic multipole moments are key concepts describing electromagnetic orders of materials. In classical theory, by coarse-graining the microscopic ones, we can define macroscopic multipole moments and reveal their characteristics clearly. For example, it is well known that the electric polarization produces charges at the edges of materials, while its spatial divergence contributes to bound charges in the bulk. Despite their theoretical importance, it was difficult to formalize electromagnetic multipole moments in crystals as bulk quantities, even the dipole moments, in quantum mechanics. This problem was solved by the modern theory of polarization, and it was found that the polarization current is given by the Berry curvature in the time and wavenumber space. Since then, the relationship between a geometric property of the Bloch wavefunction and electromagnetic multipole moments has been studied intensively.

While spontaneous electromagnetic orders appear in materials, they can be induced by applying an external field or by breaking symmetries. One of such phenomena is a magnetoelectric effect, in which the magnetization emerges in response to the applied electric field and the electric polarization emerges in response to the magnetic field. It was theoretically proposed and confirmed experimentally more than a half century ago, and has been attracting much attention in the field such as multiferroics and topological phases. On the other hand, perturbation that leads to spatial inhomogeneity, such as strain and strain gradient, also induces electric polarization and magnetization. We can introduce spatial inhomogeneities by various ways and consider a wide range of responses as well, in which profound insights into new physical phenomena can be found. Therefore, theoretical understanding for responses to general inhomogeneity is desirable, and it is also important to demonstrate the validity of the theory via model calculation for an experimental realization. Stimulated by these motivations, we construct a general theory for physical phenomena induced by spatial inhomogeneities and carry out the demonstration of the validity.

In this thesis, we study the electric polarization, current, and spin magnetization induced by spatial inhomogeneity by the Kubo formula. First, we derive an expression for the electric polarization in inhomogeneous crystals. We introduce the inhomogeneity linear in the spatial coordinates and calculate the polarization up to the first order in spatial gradient of the inhomogeneity. We assume that the perturbation has the same crystallographic translation symmetry as the unperturbed Hamiltonian, and it enables us to express the polarization induced by spatial inhomogeneity as bulk quantity. We compare the obtained formula with the one derived by the semiclassical theory, and find that they are different. Remarkably, we find

a new term which is absent in the previous work. In order to verify the additional term that we find, we introduce a two-dimensional tight-binding model and calculate the charge density in inhomogeneous crystals both by the direct diagonalization and by analytical formula. The results imply that the charge density includes the new contribution of the polarization that we find. We also note that our formula lacks the topological term in the polarization induced by spatial inhomogeneity because it is in the second order in the spatial inhomogeneity.

Next, we derive a formula for the spin magnetization in inhomogeneous crystals. The procedure of its derivation is similar to that for the polarization, and we obtain a multi-band formula for the spin magnetization induced by spatial inhomogeneity. Owing to our formula, we can directly calculate the spin magnetization in inhomogeneous crystals with band degeneracies. We also show that our result agrees with the previous work on the spin magnetization in nonuniform crystals calculated by the gradient expansion of the Keldysh Green's function. Furthermore, in order to demonstrate the validity of our formula, we consider a one-dimensional spinful tight-binding model and introduce two kinds of inhomogeneities; the spatial modulation of an on-site potential and that of the hopping amplitudes. We calculate the spin magnetization induced by the inhomogeneities both by the direct diagonalization and by our formula. By comparing their results, we see that our formula well describes the spin magnetization in inhomogeneous crystals.

Finally, we study the electric current in inhomogeneous crystals in order to clarify the physical mechanism of phenomena induced by spatial inhomogeneity. First, we calculate the inhomogeneity-induced current for insulators at zero temperature based on our formalism, and show that it is a purely magnetization current, due to spatial variation of the orbital magnetization. Next, we calculate the current in inhomogeneous metals with disorder at arbitrary temperature in the static limit, by incorporating the disorder effect as a self energy of the Matsubara Green's function. In metals, the current induced by inhomogeneity may have Fermi surface terms which might be affected by disorder scattering. We find that the inhomogeneity-induced current is purely a magnetization current and does not depend on the relaxation time even for metals with disorder, which is naturally expected for physical quantities in the static limit. We also calculate the spin magnetization in inhomogeneous metals with disorder in the static limit, and show that it is also of an intrinsic origin.

Publication List

Publication relevant to this thesis

1. N. Arai and S. Murakami,
   "Theory of Spin Magnetization in Inhomogeneous Crystals"
   J. Phys. Soc. Jpn. **94**, 034701 (2025).

Other publication

1. N. Arai and S. Murakami,
   "Anisotropic Penetration Depths of Corner States in a Higher-Order Topological Insulator"
   J. Phys. Soc. Jpn. **90**, 074711 (2021).