論文の要旨

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論文題目　Development of the Magnetic-Field-Containing Relativistic Tight-Binding Approximation Method: Revisiting the de Haas-van Alphen Effect
（磁場を含んだ相対論的強束縛近似法の開発：ド・ハースーファン・アルフェン効果の再考）

The de Haas-van Alphen (dHvA) effect is an oscillatory behavior of the magnetization as a function of the magnetic field. Measurements of the dHvA effect are widely used to probe the geometry of the Fermi surface, the cyclotron effective mass and the scattering lifetime of the conduction electrons. A conventional theory for the dHvA effect was developed by Lifshitz and Kosevich (LK) in 1956, which is called LK formula. The LK formula is based on both the Bohr-Sommerfeld quantization rule and the semi-classical equation of motion for the Bloch electron in the presence of the magnetic field. Namely, the LK formula is not derived by solving the Schrödinger or Dirac equation for the electron in both periodic potential and magnetic field. However, unfortunately, it has been difficult to solve them directly up to the present.

In this thesis, we developed the magnetic-field-containing relativistic tight-binding (MFRTB) approximation method, which is the first principles calculation method for electronic structures of materials immersed in the uniform magnetic field. In this method, both magnetic field and relativistic effects are taken into consideration by treating the Dirac equation for an electron that moves in the both magnetic field and periodic potential of a crystal.

In this thesis, we apply MFRTB method to two-dimensional square lattice model with only *s*-electrons to check the validity. It is shown that if the Zeeman term is neglected, then the MFRTB method reproduces the magnetic-field-dependent energy diagram that is so-called Hofstadter's butterfly diagram. If the Zeeman term is taken into consideration as it should be, then the magnetic-field-dependent energy diagram is split into two parts due to the spin Zeeman effect. Thus, it is shown that the MFRTB method is the generalized method that includes the Hofstadter's method.

Next, in order to check the applicability of the MFRTB method to realistic materials, we apply the MFRTB method to the crystalline silicon immersed in the uniform magnetic field. We successfully revealed E-$\boldsymbol{k}$ curves of the crystalline silicon immersed in the uniform magnetic field at the first time. Furthermore, recursive structures in the magnetic-field-dependent energy diagram, i.e., the butterfly patterns, can be seen in the k_x-k_y plane in the magnetic first Brillouin zone, but due to the k_z

dependence of the energy bands, such characteristic structures disappear in the magnetic field dependent energy diagram. It is also found from the magnetic-field-dependence the energy band width that the useful range of the effective mass approximation, which leads to the Landau levels, is limited to the region of the low magnetic field.

Finally, we apply MFRTB method to the simple cubic lattice immersed in the uniform magnetic field in order to revisit the dHvA effect by means of MFRTB method. Oscillations of the total energy and magnetization (dHvA effect) with the inverse of the magnetic field are revisited directly through the MFRTB method. It is shown that the conventional LK formula is a good approximation to the results of the MFRTB method in the experimentally available magnetic field (9.8T to 46T). The MFRTB method is capable of becoming a useful method to describe the magnetic oscillations without assumptions contained in the LK formula. Furthermore, the additional oscillation peaks of the magnetization are found especially in the high magnetic field, which cannot be explained by the LK-formula. This additional magnetic oscillation peaks may come from the fine structure of E-$\boldsymbol{k}$ curves, which is first time revealed through the MFRTB method.

The present work may become an important milestone toward revisiting the dHvA oscillations of more realistic lattice structures by means of the MFRTB method. For example, when we apply the MFRTB method to more realistic lattice structures, magnetic oscillations will be obtained in a similar way to the present case (a simple cubic lattice). Namely, by reference to the above-mentioned knowledge obtained from the present work, the LK formula is expected to give a good approximation for the period of the main oscillation in the low magnetic field region. Therefore, if there is a discrepancy between the period that is calculated by the MFRTB method and that of the LK formula, it can be concluded that this discrepancy comes from the error of the extremal cross-section of the Fermi surface. Also, if additional fine oscillations besides the main oscillation are observed in experiments, we can say that such fine oscillations do not always come from the errors of the extremal cross-section of the calculated Fermi surface but may come from the fine structures of E-$\boldsymbol{k}$ curves obtained from the MFRTB method.