論文の要旨
（Thesis Summary）

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論文題目(Thesis Title)

A Theoretical Study on the Mechanism for the Reduction of Effective g-factor in Graphene (グラフェンにおける有効g因子の減少のメカニズムに関する理 論的研究)

Graphene is a remarkable material in the field of electronic and spintronic due to its unusual properties in a magnetic field. Such astonishing properties are strong orbital diamagnetism, unconventional oscillation of magnetization, and half integer quantum Hall effect. Recently, the reduced effective g-factor has been observed in graphene by the electron spin resonance (ESR) experiments. The observed effective g-factor is about 3.1 percent smaller than that of a free electron (g=2.0023). Since the effective g-factor is the key-quantity on determining magnetic properties of materials such as the spin relaxation time, the reduction of effective g-factor has received a lot of attention in recent years.

This thesis is aimed at theoretically elucidating the mechanism of the reduced effective g-factor in graphene. As one of the causes, it is expected that both the bulk spin-orbit (SO) interaction and the internal magnetic field induced by the strong orbital diamagnetism might affect on the splitting ~~of~~ between the highest occupied state (HOS) and the lowest unoccupied state (LUS) (HOS-LUS gap) in graphene. These may cause the reduction of the effective g-factor in graphene. Hence, in this thesis, the nonperturbative magnetic-field-containing relativistic tight-binding approximation (MFRTB) method is applied to graphene immersed in a magnetic field to elucidate the mechanism of the reduced effective g-factor in graphene. It is found that there is no dependence of the bulk SO interaction on the external magnetic field. This implies that the bulk SO interaction does not effect on the effective g-factor. It is also shown that the magnetic field induced by strong orbital diamagnetism is one of the reasons for reduction of the effective g-factor. Specifically, the estimated effective g-factor of graphene is 1.986 when the external magnetic field is 1 T, which is a reduction of about 0.7 percent. This, however, does not fully account for the magnitude of the reduction in the g-factor of graphene observed in previous experiments.

In the calculations by the nonperturbative MFRTB method, the existence of the substrate, which causes the Rashba effect due to the breaking of the space inversion symmetry, is ignored. So, we carried out our calculation on effective g-factor using empty lattice model to investigate the effect of Rashba effect on the reduction in effective g-factor. Rashba effect gives rise to the additional Hamiltonian that is so called as the Rashba Hamiltonian and modifies the energy spectrum of the electrons and introduces a splitting on the electronic band. Precisely, the work function causes the asymmetric potential. Due to Rashba effect, this asymmetric potential causes magnetic field which is in-plane direction of the graphene sheet. This magnetic field is coupled with the spin magnetic moment, which forms a kind of SO interaction. In order to investigate this mechanism, we derive an expression for the HOS-LUS gap and then use thus-obtained energy splitting to evaluate the effective g-factor. The calculation from our model system shows that the reduction in effective g-

factor is 3.6 percent. This means that the Rashba effect is the primary cause for the reduction in the g-factor. Due to Rashba effect, the spin magnetic moment tilts towards the in-plane direction of the graphene sheet in the presence of external magnetic field applied perpendicular to the graphene sheet. This tilting of spin magnetic moment depends on strength of Rashba effect. As a result, the external magnetic field appreciably decreases the energy splitting. This leads to a reduction in the observed g-factor in the graphene sheet. Hence, Rashba effect could be another potential source for the reduction of the g-factor in graphene.

Furthermore, we have reformulated the MFRTB method to incorporate the Rashba effect. Numerical calculations are our future work. It is expected that we may estimate the reduction in g-factor of graphene more correctly. This could be a gateway to enhance the calculation scheme to re-evaluate the diamagnetism of graphene and to get near numerical agreement with the experimentally recorded value of the g-factor of graphene.

Finally, we shall give a comment on the significance of this work. Since the g-factor determines the spin relaxation time, it has been a major topic of interest in the field of spintronics. As a result, new findings in this thesis can be used as a guideline when designing spintronics devices. In addition, Rashba effect may produce the reduction of effective g-factor in various atomic layer materials. For instance, the opening of the energy band gap in bilayer graphene makes it appealing for application areas. Rashba effect induced by the surface potential in bilayer graphene may be similar to that in monolayer graphene. Therefore, the results of this research can be used as a general reference when looking into the effective g-factor of atomic layer materials.