Summary of Dissertation

Title: Theoretical Study of the Quantized Hall Conductivity in Graphene by using Nonperturbative Magnetic-Field-Containing Relativistic Tight-Binding Approximation Method

(非摂動論的磁場を含んだ相対論的強束縛近似法によるグラフェンの量子化されたホール伝導度に関する理論的研究)

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Recently, graphene has become a promising material as a monolayer in the electronic and spintronics fields for its extraordinary energy band diagram. Graphene in a uniform magnetic field shows some excellent properties such as strong orbital diamagnetism, unconventional oscillation of magnetization, reduced effective g-factor, half-integer quantum Hall effect (QHE), etc, due to the high mobility charge carriers for the linear energy dispersion relationship near the Dirac point. The half-integer QHE in graphene has become more attractive after theoretical predictions [1] and experimental discoveries [2,3]. But a description based on the first principle calculation has not been made yet. For this reason, a novel description of the motion of magnetic Bloch electrons in graphene immersed in a uniform magnetic field is explained in order to describe the QHE using the nonperturbative Magnetic-Field-containing Relativistic Tight-Binding (MFRTB) approximation method. This nonperturbative MFRTB method has been developed for the better description of the properties of materials immersed in a uniform magnetic field [4,5]. This nonperturbative MFRTB method enables to calculate the electronic band structure taking a periodic potential of crystal and relativistic effects into consideration.

In this study, the theoretical calculations are performed in order to investigate the QHE in graphene based on the calculated magnetic energy band structure using the nonperturbative MFRTB method [6]. For this aim to investigate the QHE in graphene, the Hall conductivity, σ_{Hall} is measured by using Streda formula [7]. For this reason, the Fermi energy dependence of the σ_{Hall} is investigated using the nonperturbative MFRTB method.

The dependence of σ_{Hall} on the position of the Fermi energy is calculated for various magnitude of magnetic fields by using the nonperturbative MFRTB method. The nonperturbative MFRTB method successfully revisited the two sets of plateaus for the quantized σ_{Hall} with filling factors (FFs) of 2, 6, 10, 14 etc., and with 0, 4, 8, 12 etc (Fig.1). The former is characterized by a wide plateau (WP), and the latter by narrow plateau (NP). In order to describe these two sets of quantized σ_{Hall}, the magnetic-field dependence of energy spectrum of electrons using the nonperturbative MFRTB method is calculated. This magnetic-field dependence of energy spectrum is well known as the Hofstadter butterfly diagram [8]. The nonperturbative MFRTB method explored two types of energy gap (Fig.2); one is characterized by a large energy gap. This large energy gap corresponds to the Onsager's area quantization of the electron orbit, which represents the behavior of the square root of the magnetic field which is first predicted by McClure [9,10]. Another is characterized by a small energy gap which is due to the relativistic effects, mainly the spin-Zeeman effect and spin-orbit interaction. It is found that these two types of energy gap are the origins of observed two types of plateaus. That is the WPs and NPs are attributed to the large energy gap and small energy gap, respectively.

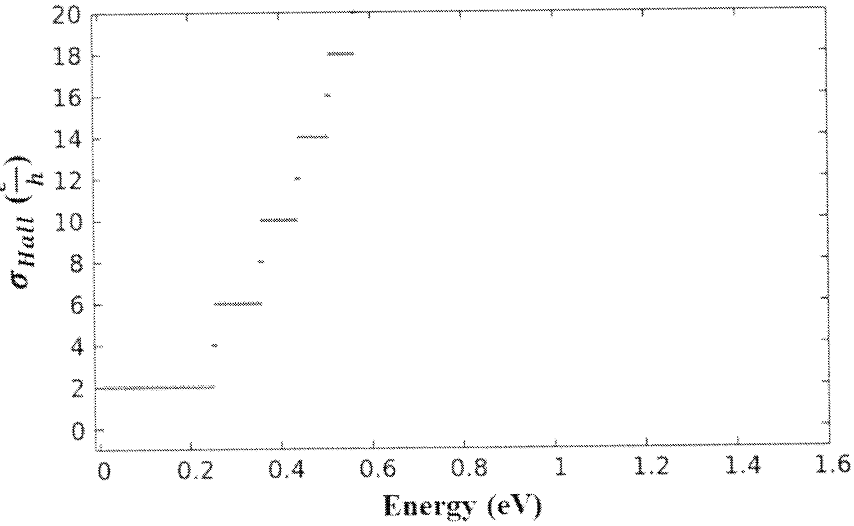

Fig. 1: Fermi energy dependence $\sigma_{Hall}(e^2/h)$ for 48.50 (T).

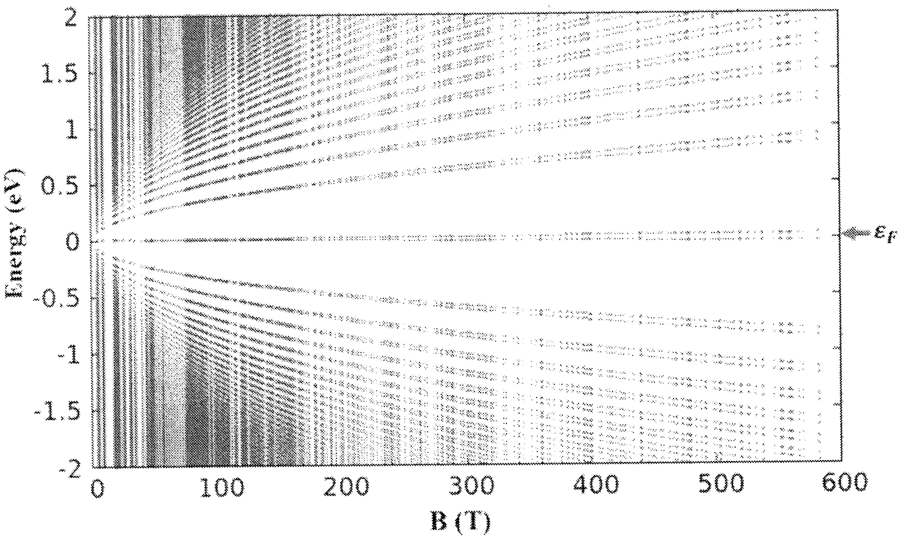

Fig. 2: Magnetic field dependence energy spectrum.

While the WPs corresponds to the energy gaps related to the Onsager's area-quantization rule, the NPs corresponds to the energy gaps caused by relativistic effects such as the Zeeman spin effect and spin-orbit interaction. The widths of both plateaus depend on the magnetic field, which can also be explained based on the magnetic energy band structure. Thus, it is shown that the magnetic energy band structure can successfully explain the quantized σ_{Hall} in graphene immersed in a uniform magnetic field.

In this study, the Fermi energy dependence of the widths of WPs and NPs is investigated in detail. The width of WPs decreases with Fermi energy for a constant magnetic field (Fig.3), which is same as the experimental results [2,3]. In the lower-energy region, the dependence of the width of WPs is more consistent with the result of the conventional theoretical model [9,10]. This consistency appears in the lower energy region near the Dirac point where the linear energy dispersion relationship approximation for the energy band structure in the absence of a magnetic field holds. On the other hand, in the higher-energy region, the result of the nonperturbative MFRTB method does not coincide with the conventional theoretical model This is because the conventional theoretical model is valid only for the linear energy dispersion relationship which appears near the Dirac point or low energy region. On the other hand, the nonperturbative MFRTB method is valid both in the lower and higher energy regions. The nonperturbative MFRTB method provides a realistic magnetic energy band structure in the both energy regions. For this reason, the discrepancy appears due to the lack of validity of the linear energy dispersion relationship in the higher-energy region. The Fermi energy dependence of the width of WPs calculated by the nonperturbative MFRTB method is more reliable in both the lower and higher energy regions.

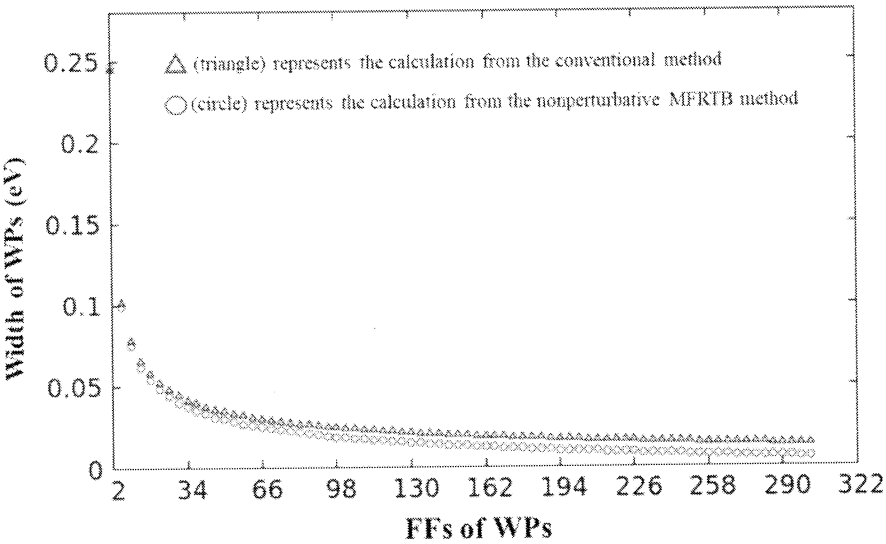

Fig. 3: Filling factor dependence width of WPs for 48.50 (T).

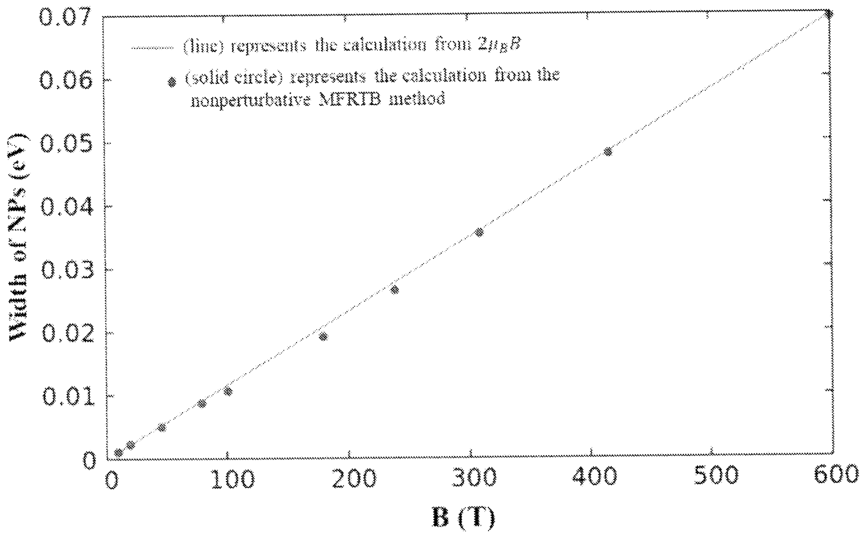

Fig. 4: Magnetic-field dependence width of the NP for the FF=4.

As mentioned above, the width of the NPs using the nonperturbative MFRTB method is attributed due to the spin-Zeeman effect and spin-orbit interaction. Note that only the spin-Zeeman effect is taken into consideration in the conventional model. The calculation results of the conventional model and the nonperturbative MFRTB method good coincide in the low and high magnetic field case but not coincide in the middle magnetic field case (Fig.4). If the spin-orbit interaction is neglected, the NPs are attributed only due to the spin Zeeman effect. So, the width of NPs coincides with the width expected from the spin-Zeeman effect.

In the high magnetic field region, the spin-Zeeman effect is more dominant part compared to the spin-orbit interaction part. For this reason, the calculated width of NPs using the nonperturbative MFRTB method is nearly the same as the calculated width of NPs by the spin-Zeeman effect. So, in this region, the effects of the spin-orbit interaction become negligible compared to the spin-Zeeman effect, which is known as the Paschen–Back effect.

In the low magnetic field region, the spin-Zeeman effect is less dominant part compared to the spin-orbit interaction part. So, the spin-orbit interaction would be expected as a dominant part. The difference, should be large, it is expected. However, the calculation using the nonperturbative MFRTB method coincides with the result of the conventional model for an FF of four. This agreement is explained in the following as, in this region for this FF of four (4), the agreement indicates that the energy splitting caused by the anomalous Zeeman effect is consistent with that of the spin-Zeeman effect for the magnetic Bloch states. This agreement for a particular FF is possible, for example, when the magnetic quantum number of the total angular momentum is given by $\pm 1/2$, the energy splitting caused by the anomalous Zeeman effect is consistent with that caused by the spin-Zeeman effect in a low magnetic field. This agreement in the low magnetic field region implies that the magnetic Bloch states related to FF of four mainly comprise atomic orbitals with the magnetic quantum number of $\pm 1/2$.

In the middle magnetic field region, the difference is comparatively large. The spin-Zeeman effect and the spin-orbit interaction both are the dominant part. For this reason, the discrepancy is comparatively large in the middle magnetic field region (approximately 200 (T)). This result suggests that the width of NPs in a magnetic field of approximately 200 (T) can be affected due to the effect of the spin-orbit interaction in graphene. This effect provides very important information in research in graphene around this magnetic field.

It is possible to observe the effect of the spin-orbit interaction and Paschen–Back effect in graphene by investigating the Fermi energy dependence of the width of NPs at magnetic fields greater than 100 (T).

References

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