論文の内容の要旨

論文題目： Gauge theory for phase structure of honeycomb lattice

（蜂の巣格子上でのゲージ理論による相構造）

氏名： 荒木 康史

Graphene is a monoatomic layer material composed of carbon atoms, arranged in the honeycomb lattice structure. It has been studied intensely as a two-dimensional electronic system easy to create and observe, since its first experimental isolation by Geim and Novoselov in 2004. Charge carriers on monolayer graphene can be described as massless Dirac fermions at long wavelength limit in the vicinity of two "Dirac points" in the momentum space, known as the "Dirac cone (valley)" structure. This nature makes graphene attractive from the viewpoint of quantum field theories as well as of materials physics.

However, the Dirac cone picture may break down in the presence of a strong electron-electron interaction, where the excitations are more likely to be scattered to the momentum region far from the Dirac cones. Such a strong coupling is supposed to be achieved in a vacuum-suspended graphene, where the Coulomb interaction is effectively enhanced from the ordinary quantum electrodynamics (QED), by the discrepancy between the propagation speed of the charge carriers (Fermi velocity, $v_F=c/300$) and that of photons (speed of light, c). Under such a strong electron-electron interaction, some symmetry of the system may get spontaneously broken, driving the system into an excitonic insulator. This mechanism is analogous to the spontaneous breaking of chiral symmetry and dynamical fermion mass generation in strongly coupled field theories, such as quantum electrodynamics (QCD). In graphene, however, its microscopic lattice structure may host various gap-opening patterns (see Fig.1):

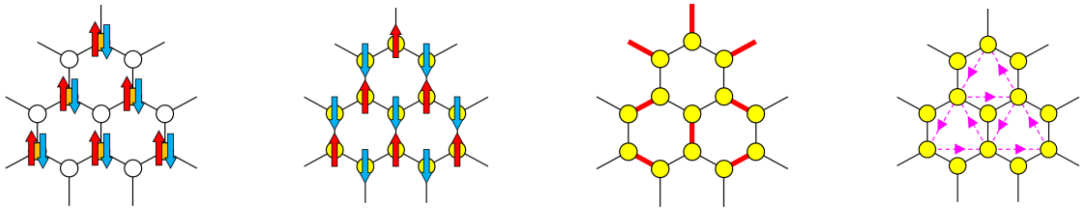
(a) **Charge density wave (CDW)**: One triangular sublattice of the honeycomb lattice is more occupied by electrons than the other sublattice. It breaks the discrete chiral symmetry defined by two sublattices. It can be induced explicitly by some external substrates, like silicon carbide or boron nitride.

(b) **Spin density wave (SDW)**: One sublattice is occupied by electrons with a certain spin direction, while the other sublattice by the opposite spin direction. The system shows antiferromagnetism. It breaks both the sublattice symmetry and the spin SU(2) symmetry.

(c) **Kekulé distortion**: Nearest-neighbor hopping amplitude becomes non-uniform with a certain pattern larger

than the unit cell, breaking the translational invariance partially. It can be induced explicitly by some adatoms on the layer.

(d) **Haldane/Kane-Melé flux**: Next-to nearest neighbor hopping with a complex amplitude is induced by an effective "magnetic flux", breaking the time-reversal symmetry. Haldane flux preserves the SU(2) spin symmetry, inducing an anomalous quantum Hall conductivity. Kane-Melé flux, which breaks the spin symmetry, corresponds to spin-orbit interaction, and induces a so-called "quantum spin Hall" effect.



(a) (b) (c) (d)

Fig.1: Schematic picture of the gap-opening orders characteristic to the honeycomb lattice.

The interplay among these ordering patterns, induced either spontaneously or externally, is still little known under the sufficiently strong electron-electron interaction. Motivated by those problems in monolayer graphene, we study the phase structure of graphenelike systems with a sufficiently strong electron-electron interaction in this thesis. We assume that the interaction is mediated by the electromagnetic field like quantum electrodynamics (QED), and investigated the interplay effects among various ordering patterns (either spontaneous or explicit) listed above.

In Section 2, we construct a lattice gauge theory model defined on the graphenelike honeycomb lattice. We convert the conventional tight-binding Hamiltonian into path integral formalism, and define the lattice effective action, with the effect of electron-electron interaction included in terms of U(1) gauge field. This is the lattice gauge theory description of the so-called "reduced QED", where the fermions are confined in the (2+1)-dimensional plane, while the photons (gauge field) propagate in the (3+1)-dimensional space. This effective model can host the ordering patterns shown above, which are characteristic to the honeycomb lattice, except for those preserving the full SU(2) spin symmetry.

In the first half of Section 3, we observe the phase structure of the graphenelike gauge theory constructed above by using the techniques of strong coupling expansion of lattice gauge theory, inspired by the analyses of QCD phase structure. Strong coupling expansion decomposes the long-range Coulomb interaction into the sum of 4-fermi local interaction terms. The leading order in the expansion gives the on-site interaction, which may lead to the spontaneous sublattice symmetry breaking (SLSB), while the next-to leading order yields the nearest-neighbor repulsion, which can contribute to the renormalization of the Fermi velocity and

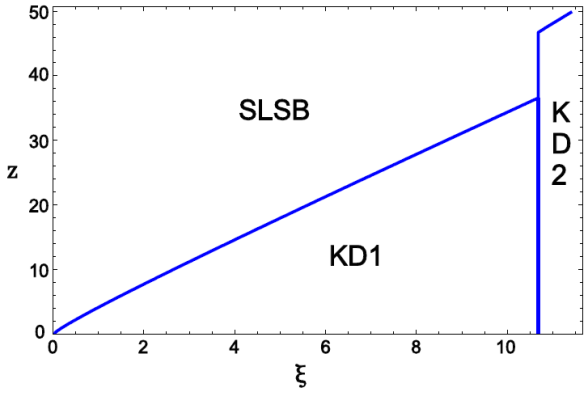


Fig.2: Phase diagram displaying the competition among spontaneous orders: SLSB, KD1 and KD2. Vertical axis represents the strength of leading order (on-site interaction), while the horizontal axis the next-to leading order (nearest neighbor repulsion).

the spontaneous Kekulé distortion. We map the phase diagram of the system with these spontaneous orders at the mean-field level, by varying the ratio between the amplitudes of terms in the expansion (see Fig.2). It should be noted that the Kekulé distortion is classified into two phases (KD1/KD2), characterized by the sign of its amplitude. The difference of two Kekulé distortion phase originates from the parabolic band far from the Dirac points, which is neglected in the Dirac cone approximation.

In the second half of Section 3, we focus on the competition between the spontaneous sublattice symmetry breaking seen above and the externally introduced orders, within the strong coupling limit of lattice gauge theory. Here we incorporate Kekulé distortion and Kane-Melé flux (spin-orbit interaction) as the explicit orders. In the presence of a sufficiently large Kekulé distortion, the spontaneous order is suppressed and the sublattice symmetry gets restored, which agrees with the analysis within the Dirac cone approximation. On the other hand, when the distortion amplitude is small enough, the sublattice symmetry breaking order grows quadratically as a function of the distortion amplitude, which cannot be seen within the Dirac cone approximation (see Fig.3). Therefore, microscopic effect from the lattice structure is crucial for the interplay of these orders, as long as the Kekulé distortion amplitude is small compared to the energy scale characterized by the lattice structure.

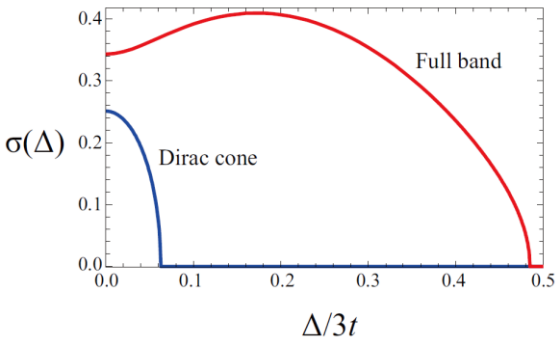


Fig.3: Behavior of spontaneous SLSB order σ(Δ) in the presence of the external Kekulé distortion Δ. "Full band" is calculated with the full band structure, while "Dirac cone" is obtained by Dirac cone approximation.

The spin-orbit interaction, which breaks the sublattice symmetry, SU(2) spin symmetry, and the valley (pseudospin) inversion symmetry, also competes with the spontaneous antiferromagnetic order, which breaks the sublattice and spin symmetry but preserves the valley inversion symmetry. The spin-orbit coupling tilts the antiferromagnetic order towards the XY-plane, away from the direction originally pointed by the spin-orbit term. Such an interplay between the normal antiferromagnetic order and the spin-orbit coupling occasionally shifts the topological phase structure of the system, which can contribute to quantum spin Hall effect (see Fig.4). This phase structure is also related with the parity-breaking phase of lattice QCD with Wilson fermions, which is called "Aoki phase". We can give a conjecture about the phase structure of quantum spin Hall system at finite coupling, from the analogy with the phase structure of lattice QCD.

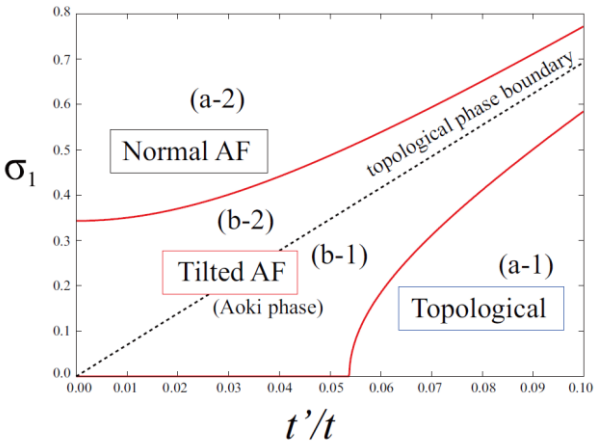


Fig.4: Phase diagram in the presence of spin-orbit coupling (t') and the normal antiferromagnetic (AF) order (σ_1). There appears a new "tilted AF" phase by the effect of electron correlation.

In Section 4, we attempt to give a clue about the breaking/restoration of the exact SU(2) spin symmetry in the honeycomb lattice system, which cannot be observed in the lattice gauge theory due to the artifact of lattice discretization. Here we employ the extended Hubbard model, which includes the 4-point interaction terms similar to those derived from the strong coupling expansion of lattice gauge theory. We observe the phase structure of this model by solving the variational gap equations including CDW and SDW orders. Variational gap equation, which is optimized on the basis of Jensen-Peierls inequality, is advantageous over the ordinary mean-field gap equation derived by Hubbard-Stratonovich transformation in that competition among various order parameters can be taken into account. In the absence of the external staggered potential, the phases are classified into CDW, SDW, and semi-metallic phases. The on-site (Hubbard) repulsion favors SDW, while the nearest-neighbor (NN) repulsion favors CDW. The external staggered potential enhances the CDW phase, suppressing the SDW phase (see Fig.5). The spin SU(2) symmetry is broken in the SDW phase, and the band degeneracy of two spin states is correspondingly shifted in the presence of the external staggered potential: band gap amplitudes and Fermi velocities of the electrons with up/down spin become different (see Fig.6). This phenomenon may have an effect on the spin transport, such as the filtering of spin components.

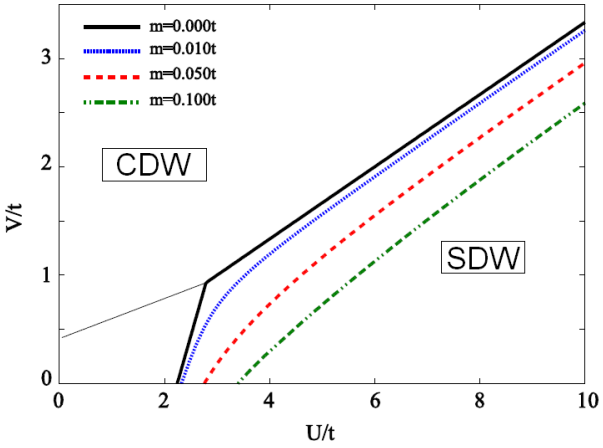


Fig.5: Phase diagram of the extended Hubbard model, with the on-site (Hubbard) repulsion *U* and the NN repulsion *V*. External staggered potential *m* eventually suppresses the SDW phase.

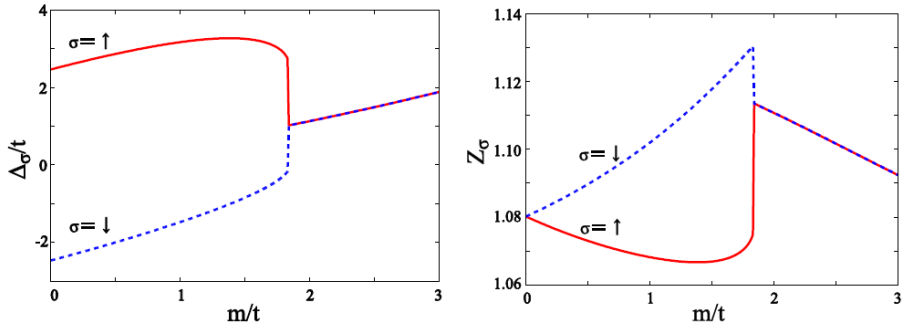


Fig.6: Behavior of the gap amplitude Δ_σ (left) and the Fermi velocity renormalization factor Z_σ for each spin state $\sigma = \uparrow, \downarrow$, as functions of the external staggered potential m, where the on-site interaction U=6.0t and the NN interaction V=0.5t. Band degeneracy is shifted in the SDW phase.

We expect that all the analytical results above can be tested experimentally by the direct observation of band structure like angle-resolved photoemission spectroscopy (ARPES), or the measurement of electronic transport properties like charge/spin Hall effects. Our results can be applied to the correlated fermion systems on the honeycomb lattice, such as graphene, cold atoms on optical lattice, and the topological insulators, with a small modification. The application of our methods to the bilayer graphene systems, where the spontaneously gapped phase has already been observed experimentally, is a future problem.