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Theoretical Exploration of Novel Topological States
（新規トポロジカル状態の理論探索）

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論　文　の　要　旨

The discovery of the quantum Hall effect (QHE) in two-dimensional (2D) electron gases by von Klitzing opened a new chapter in condensed matter physics. The underlying mechanism for exact quantization of Hall conductance was understood phenomelogically from perspectives of gauge invariance and edge currents in a finite sample. A relationship between the quantized Hall conductance and nontrivial bulk topology of Bloch wave functions was later revealed in the TKNN theory, where integer coefficient in the Hall conductance is the Chern number evaluated from the Bloch wave functions. A one-to-one correspondence between the two theories was clarified by Hatsugai, known as bulk-edge correspondence. One necessary condition for achieving the ordinary QHE is the application of strong external magnetic field. It was then shown by Haldane that the condition can be exempted in a 2D honeycomb lattice with complex next-nearest-neighbor (NNN) hopping integrals taken into consideration, which yielded the quantum anomalous Hall effect (QAHE) . Due to broken time-reversal (TR) symmetry, both QHE and QAHE are classified as Chern insulators, which can support chiral edge states. A breakthrough took place in 2005 when Kane and Mele demonstrated that the intrinsic spin-orbit coupling (SOC) in the monolayer graphene can generate the complex NNN hopping integrals, and drives the system into a quantum spin Hall effect (QSHE) preserving TR symmetry. The QSHE is characterized by a Z_2 topological invariant and can support helical edge states. While to observe QSHE in graphene is almost impossible due to the extremely small SOC, a larger gap 2D

topological insulating state hosted by HgTe quantum wells was theoretically studied and experimentally confirmed.

In the thesis, we focus on possible topological states in photonic crystals, semiconductors and superconductors including both theories and material designs. We start from the topological photonics. Photonic crystals are analogues of conventional crystals with atomic lattice replaced by a medium of periodic electric permittivity and/or magnetic permeability. Because of the periodicity in space both Bloch theorem and topological considerations apply to photonic crystals as well. A honeycomb lattice of 2D cylindrical dielectric rods can support Dirac cones at the K(K') points, which are the corner of the first Brillouin zone for honeycomb lattice. Breaking the TR symmetry by introducing the magneto-optic effect into honeycomb lattice, the system is driven into a topological phase under an external magnetic field. The resultant topological state can be regarded as an optical analogue of the ordinary QHE. In this thesis, without requiring any external field, we derive a 2D Z_2 topological photonic state purely based on conventional dielectric materials. Starting with a honeycomb lattice of cylinders, we group them into a triangular lattice of cylinder hexagons, which can support double Dirac cones at the Γ point. Detuning the lattice constant of the triangular lattice, we realize a Z_2 topological photonic state with bulk band gap opened at the Γ point. We show that the photonic topology is associated with a pseudo-TR symmetry constituted by the TR symmetry respected in general by Maxwell equations and the C_6 crystal symmetry upon design, rendering the Kramers doubling in the present photonic system. We prove for the transverse magnetic mode that the role of pseudospin is played by the angular momentum of the wave function of the out-of-plane electric field. We solve Maxwell equations and demonstrate the new photonic topology by revealing pseudospin-resolved Berry curvatures of photonic bands and helical edge states characterized by Poynting vectors. With simple design backed up by the symmetry consideration, the present topological photonic crystal can be fabricated easily, and is expected to leave strong impacts on topological photonics and related materials science.

We generalize the above idea to electronic systems. Starting with a honeycomb lattice and viewing it as a triangular lattice of hexagons, we propose a Z_2 topological state by simply enhancing the inter-hexagon hopping energies over the intra-hexagon ones. We reveal that this manipulation opens a bulk gap in the energy dispersion at the Γ point and drives the system into a Z_2 topological state. The size of the topological gap is proportional to the difference of the inter- and intra-hexagon hopping energies, which can be larger than the typical value of SOC in graphene by orders of magnitude and potentially renders topological electronic transports available at high temperatures. For experimental implementations, we discuss that, along with many other possibilities, the molecular graphene with carbon monoxides (CO) placed periodically on Cu [111] surface is a very promising platform to realize the present idea, where the hopping texture can be controlled by adding extra CO molecules.

Breaking both TR and inversion symmetries we propose a novel QAHE characterized by simultaneous charge and spin Chern numbers, which can support non-dissipative spin-polarized edge current in a finite sample. We revealed that this novel QAHE can be realized in a buckled honeycomb lattice with anti-ferromagnetic (AFM) exchange field at two sublattice sites, intrinsic SOC and tunable electric field. The novel QAHE is achieved when magnitudes of these three fields satisfy the triangle condition, namely summation between any two is larger than the remaining one. By performing first-principles calculations, we have shown that a G-type AFM Mott insulator $LaCrO_3$ grown along the [111] direction with one layer of Cr atom replaced by Au or Ag can support the novel QAHE. Considering that synthesizing the system along the [111] direction is not an easy task, we also propose a sandwiched structure composed of the $LaCrO_3$ grown along the [001] direction with one atomic layer replaced by an inverse perovskite material Sr_3PbO. Based on first-principles calculations we confirm that the system should demonstrate the novel QAHE, which is consistent with numerical results of nonzero charge and spin Chern numbers as well as spin-polarized edge states. Since these two materials in the second proposal are stable in bulk and match quite well with each other, the composite material is expected easy to synthesize. This novel QAHE with non-dissipative spin-polarized edge currents is robust to both non-magnetic and magnetic defects, and is thus ideal for spintronics applications.

An important and promising application of topological states is the decoherence-free topological quantum computing. Majorana fermion (MF), a zero-energy quasi-particle in topological superconductors that is its own anti-particle, is the key to realize the expected novel quantum functionalities. We study the topological superconductivity in a heterostructure composed of a ferromagnetic insulator, a semiconductor with strong Rashba SOC and an s-wave superconductor with vortices. It was shown before that the non-Abelian statistics can be achieved by exchanging the positions of two vortices hosting MFs. However, in experiments it is difficult to manipulate vortices. In order to circumvent this difficulty, we propose a new way to interchange MFs without moving vortices. The only operation required is to turn on and off local gate voltages, which liberates a MF from its original host vortex and transports it along prepared tracks. We solve the time-dependent Bogoliubov-de Gennes equation numerically, and confirm that the MFs are protected when the switching processes of gate voltages are controlled to the order of nano seconds for reasonable material parameters. By monitoring the time evolution of MF wave functions, we show that non-Abelian statistics is achieved. The present scheme provides a feasible way for manipulating MFs and thus useful in future topological quantum computing.

審　　査　　の　　要　　旨

〔批評〕

本論文は、物質における新規トポロジカル性質及びその特異なエッジ状態を理論的に調べたものである。トポロジカル電磁波伝播を実現するためには外部磁場の印加や特殊な材料が必要とされていたが、本論文が誘電体でできたフォトニック結晶におけるトポロジカル特性発現を初めて解明した。フォトニック結晶の空間対称性を利用して、電磁波モードに有効的なスピン自由度を作り出し、時間反転対称性が保たれているトポロジカル電磁状態の実現方法を示した。また、二次元電子系のディラック分散関係について、スピン軌道相互作用と共に、反強磁性交換場及び交替電場による PT 対称性の破れを解析した。理論的な考察に基づいて、量子異常ホール効果を示すペロフスカイト物質のヘテロ構造を第一原理に基づいて設計し、スピン分極を持った散逸のないエッジ電流の実現方法を提案した。さらに、強靱なトポロジカル量子計算の実現を念頭に、二次元トポロジカル超伝導の量子渦にあるマヨラナ準粒子の位置交換の方法を考案し、マヨラナ準粒子が満たす非アーベル統計性を示した。これらの結果は、新規なトポロジカル状態の持つ様々な可能性の解明に寄与し、今後の実験研究の指針になりえるものである。

以上の理由から、本論文は博士論文として十分と判断された。

〔最終試験結果〕

平成28年2月12日、数理物質科学研究科学位論文審査委員会において審査委員の全員出席のもと、著者に論文について説明を求め、関連事項につき質疑応答を行った。その結果、審査委員全員によって、合格と判定された。

〔結論〕

上記の論文審査ならびに最終試験の結果に基づき、著者は博士(工学)の学位を受けるに十分な資格を有するものと認める。