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Title	Time Crystals and Space Crystals in terms of Macroscopic Quantum Phenomena [an abstract of dissertation and a summary of dissertation review]
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Degree Grantor	北海道大学
Degree Name	博士(工学)
Dissertation Number	甲第13988号
Issue Date	2020-03-25
Doc URL	https://hdl.handle.net/2115/78116
Rights(URL)	https://creativecommons.org/licenses/by/4.0/
Type	doctoral thesis
File Information	Keiji_Nakatsugawa_abstract.pdf, 論文内容の要旨



学 位 論 文 内 容 の 要 旨

博士の専攻分野の名称 博士（工学） 氏名 中津川 啓治

学 位 論 文 題 名

Time Crystals and Space Crystals in terms of Macroscopic Quantum Phenomena

(時間的結晶・空間的結晶:巨視的量子現象としての研究)

Crystals are ubiquitous around us and they have been studied extensively. However, new kinds of crystals including fullerene, carbon nanotube and topological crystals have been discovered. On the other hands, a new type of state called time crystal has been proposed: In this state, a description with macroscopic wave functions is necessary. From these backgrounds, a reconsideration of crystalline orders becomes necessary. In this thesis, I study crystalline orders in terms of macroscopic wave functions as follows:

(1) Quantum time crystal by decoherence: Physical systems can possess continuous or discrete symmetries. For example, fluids like water have continuous spatial translational symmetry, but crystals have discrete spatial translational symmetry. From the equivalence between space and time in relativity, a natural question is whether discrete time translation symmetry is possible. F. Wilczek considered this problem in terms of spontaneous breaking of time translation symmetry and proposed the idea of quantum time crystals. In this thesis, I show that time translation symmetry of a ring system with a macroscopic wave function is broken decoherence, not by spontaneous symmetry breaking. I consider a ring-shaped incommensurate charge density wave (ICDW ring) threaded by a fluctuating magnetic flux: I extend the so-called Caldeira-Leggett model to ring systems to model the fluctuating flux as a bath of harmonic oscillators. The ground state of a quantized ICDW ring without environment is a superposition of ICDWs which possess continuous space/time translation symmetry. But, as the ICDW ring couples to environment, the charge density expectation value oscillates periodically with a radius-dependent period. This model forms a metastable quantum time crystal with a finite length in space and in time. As I explain in (2), this model was realized also because of a consistent quantization of ring systems.

(2) Time Operators and Time Crystals: In quantum mechanics, position and momentum are observables (physical operators) and the position-momentum uncertainty relation is well-established. Meanwhile, uncertainty relations between time and energy are known to hold experimentally. Therefore, an important question is whether one can define time operators which can be used to derive energy-time uncertainty relations. The main difficulty is that Hermitian operators and Self-adjoint operators are different objects. Real eigenvalues and orthonormal eigenstates are ensured only for self-adjoint operators, so observables are expected to be self-adjoint. However, most of the time operators proposed so far are non-self-adjoint Hermitian operators. So, time in quantum mechanics is still regarded as a pa-

parameter. On the other hand, time crystals in (1) seem to promote time from a parameter to a physical quantity. In this thesis I consider the problem of time operators in terms of time crystals. The key ingredient is a consistent quantization of ring systems. For instance, wave functions in ring systems must satisfy periodic boundary condition, but the position operator or angle operator are multi-valued operators which violate periodicity. I show that quantization of ring systems can be understood by periodic position operators via the generalized weak Weyl relation (GWWR). Then, self-adjoint time operators in ring systems are derived based on the GWWR. In addition, I study the relationship between self-adjoint time operators and non-Hermitian operators with space-time inversion (PT) symmetry. These operators are closely related to the “temporal structure of ring systems” and they reflect the periodicity of the time crystal model in (1).

(3) Origin of Stripe and Quasi-Stripe CDW Structures in Monolayer space crystals: Layered compounds such as transition metal dichalcogenides exhibit various charge density wave (CDW) phases depending on temperature and crystal symmetry. In the conventional description of phase transition, symmetry breaking occurs as temperature decreases. However, 1T-TaS₂ (2H-TaSe₂) makes a phase transition to the triclinic phase (stripe phase) with anisotropic domain walls only when temperature is increased from the ground state. The appearance of these anisotropic phases has been explained by inter-layer interaction. However, T-domain walls were observed experimentally in monolayer 1T-TaS₂, hence a new model for the appearance of low-dimensional phases is necessary. In this thesis I used Landau theories of two-dimensional CDW phase transition to make a thorough numerical research of CDW free energy structure and discover a multivalley free-energy landscape with many local minima. In addition, I discovered local minima which correspond to the T phase and to the stripe phase. These results can be explained only by interference of macroscopic CDW wave functions, hence indicate the appearance of low-dimensional CDW phases without inter-layer interaction (hence also in monolayer). Moreover, I discussed the temperature dependence of successive phase transition, generalized the McMillan-Nakanishi-Shiba free energy theory for two-dimensional CDW phase transition, and predict the appearance of new CDW phases in 1T-TaSe₂.