（様式４）

二国間交流事業 共同研究報告書

令和 4 年 4 月 14 日

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JPJSBP1 20194828

1. 事 業 名 相手国: ロシア (振興会対応機関: RFBR)との共同研究

2. 研究課題名
（和文） 相互作用を有する空間非一様な二次元構造体
（英文） Inhomogeneous two-dimensional systems with interactions

3. 共同研究全実施期間 2019 年 4 月 1 日 ～ 2022 年 3 月 31 日 (3 年 0 ヶ月)

4. 相手国代表者(所属機関・職・氏名【全て英文】)
Institute for Theoretical and Applied Electrodynamics, Russian Academy of Science, Laboratory Head, Alexander L. Rakhmanov

5. 委託費総額(返還額を除く)

本事業により執行した委託費総額		4,712,500 円
内訳	1年度目執行経費	2,337,500 円
	2年度目執行経費	2,375,000 円
	3年度目執行経費	円

6. 共同研究全実施期間を通じた参加者数(代表者を含む)

日本側参加者等	10 名
相手国側参加者等	5 名

＊ 参加者リスト(様式 B1(1))に表示される合計数を転記してください(途中で不参加となった方も含め、全ての期間で参加した通算の参加者数となります)。

7. 派遣・受入実績

	派遣		受入
	相手国	第三国	
1 年度目	2	0	5 (0)
2 年度目	0	0	0 (0)
3 年度目	0	0	0 (0)
4 年度目			()

＊ 派遣・受入実績(様式 B1(3))に表示される合計数を転記してください。
派遣:本委託費を使用した日本側参加者等の相手国及び相手国以外への渡航実績(延べ人数)。

受入：相手国側参加者等の来日実績（延べ人数）。カッコ内は本委託費で滞在費等を負担した内数。

8. 研究交流実績の概要・成果等

(1)研究交流実績概要（全期間を通じた研究交流の目的・研究交流計画の実施状況等）

The team in Japan, and its principal investigator, Dr. F. Nori, have long-term experience in the study of quantum physics and a strong track record of publications in top physics journals. The researchers of the Russian part of the project also have extensive experience in the research fields of the project and publications in good physics journals. Our groups have collaborated very intensively since 2004. Our close collaboration in performing theoretical studies and intensive exchange of ideas allow us to complete the project at a high scientific level. The usage of the supercomputer from the Computational center of Russian Academy of Sciences allowed us to perform all numerical studies necessary for solution of the problem tasks.

The project goals focus on studies of the electronic structure of several two-dimensional, quasi-two-dimensional, and inhomogeneous systems with a nontrivial band structure, when taking into account the electron-electron interaction. Such systems include twisted graphene bilayer, Weyl semimetals, and also systems with nesting of the Fermi surface that have nontrivial electronic properties and have a tendency to display nanoscale electronic phase separation. Note that these topics have been attracting considerable attention in condensed matter physics. We also studied the effect of real Fermi surface features on the superconducting order parameter symmetry in 3D doped topological insulators. Also, we introduced the novel concept of jump-time unraveling as a distinct description of (dissipative) open quantum systems. The planned tasks were performed successfully. The results of the project were published in nine papers in very good physics journals and presented at International conferences. Moreover, we submitted several manuscripts which are posted online in the arXiv. Furthermore, we are also completing additional projects, not listed here due to space limitations.

(2)学術的価値（本研究交流により得られた新たな知見や概念の展開等、学術的成果）

During the work on the project the following tasks were solved:

1. Electronic properties of graphene bilayer with a small twist angle.

1.1. We studied the role of **many-particle effects in the electronic structure of bilayer graphene with layers rotated relative to each other** (see Ref. 1 below). Particular attention was paid to electronic characteristics at small rotation angles of the layers close to the so-called "first magic angle". In this case, the low-energy one-electron spectrum of the system consists of eight almost-flat partially degenerate zones, each of which corresponds to one electron per one unit cell of the moiré superstructure per spin projection. The weak dependence of the electron energy on the momentum makes the electronic subsystem particularly sensitive to effects of the electron-electron interaction. The degeneracy of the bands is partially removed due to this interaction, and the details of the electron spectrum become dependent on the doping level. The obtained results are consistent with experiments obtained by various experimental groups.

1.2. Near half-filling (two electrons or holes per superlattice unit), the electronic spectrum of the system loses its hexagonal symmetry and a nematic many-particle state arises (see Ref. 3 below). Manifestations of nematicity can be observed in the spatial distribution of the spin magnetization inside the moiré cell. We show that the nematicity is a stable characteristic with respect to the model parameters. The obtained theoretical results are consistent with the available experimental observations, in which the nematic state in bilayer graphene twisted at small twist angles was detected by electron spectroscopy [A. Kerelsky et al, Nature, 572, 95 (2019)].

1.3. We have also shown that i**n the concentration range where exists a set of exciton order parameters, the homogeneous state of the electron system in the twisted bilayer graphene can be unstable with respect to the phase separation** (see Ref. 5 below). Namely, the dependence of the chemical potential on doping is nonmonotonic. This result is consistent with recent experiments. Phases in an inhomogeneous state are characterized by an even number (ν = 0, ±2, ±4) of electrons per supercell. This makes it possible to explain the observed details of the conductivity behavior of the doped system under consideration.

2. Electronic phase separation in systems with nesting of the Fermi surface.

2.1. We studied the **effect of pressure on the electronic properties and phase separation in systems with imperfect nesting of the Fermi surface** (see Ref. 2 below). Nesting leads to the formation of a spin density wave (SDW). Pressure shifts the sheets of the Fermi surface, and instead of the homogeneous SDW phase, nanoscale inhomogeneities arise and a mixture of SDW dielectric and paramagnetic (PM) metal arises. The shape of the inhomogeneities depends on the volume concentration of the PM metal: initially, nanometer PM drops appear; then, cylinders and layers. Finally, at sufficiently high pressures, the system transforms into a homogeneous PM phase. We used a simple model which, nevertheless, allowed us to describe the real experimental situation in a number of low-dimensional compounds (e.g., organic metals).

2.2. At low temperatures, **fermionic systems with a perfectly nested Fermi surface orders into a spin-density wave**. Upon doping, however, the latter state becomes unstable, and several spatially inhomogeneous phases emerge competing against each other to become the true ground state. We investigate this competition using the anisotropic Hubbard model on a 3D cubic lattice in the weak-coupling regime as a convenient study case (see Ref. 8 below). For this model it is known that, at half-filling (one electron per site), the Fermi surface nesting is perfect, and the ground state is the commensurate spin-density wave. Away from half-filling, various types of spatially inhomogeneous phases, such as phase-separated states and the state with domain walls (“soliton lattice”) emerge. Using mean-field theory, we evaluated the free energies of these phases to determine which of them could become the true ground state. Our study demonstrated that the free energies of all discussed states are very close to each other. The smallness of these energy differences suggests that, for a real material, numerous factors, unaccounted by the model, may arbitrary shift the relative stability of the competing phases. We further argue that purely theoretical predictions of a structure of inhomogeneous phase in a particular doped system is unreliable.

3. New spin-valley half-metals in the systems with imperfect nesting.

A few years ago we predicted theoretically that in systems with nesting of the Fermi surface **the spin-valley half-metal has lower energy than the spin density wave state** [see A.V. Rozhkov, A.L. Rakhmanov, A.O. Sboychakov, K.I. Kugel, and F. Nori, Spin-valley half-metal as a prospective material for spin valleytronics, Phys. Rev. Lett. 119, 107601 (2017).]. We suggest a possible way to distinguish these phases experimentally (see Ref. 7 below). We calculate the dynamical spin susceptibility tensor for both states in the framework of the Kubo formalism. The phases studied have different numbers of bands: four bands in the spin-valley half-metal and only two bands in the spin density wave. Therefore, their susceptibilities, as functions of frequency, have different numbers of peaks. Moreover, the spin-valley half-metal does not have rotational symmetry; thus, in general the off-diagonal components of the susceptibility tensor are nonzero. The spin density wave obeys robust rotational symmetry and the off-diagonal components of the susceptibility tensor are zero. These characteristic features can be observed in experiments with inelastic neutron scattering.

4. Magnetoresistance of Weil semimetals.

We studied the effect of random potentials created by various types of impurities on the transverse magnetoresistance of the Weyl semimetals (see Ref. 6 below). We showed that the type of impurity potential strongly affects the magnetic field and temperature dependences of the magnetoresistance. Two limiting cases are analyzed in detail: (i) the ultraquantum limit, when the applied magnetic field is so strong that only the zero and first Landau levels participate in magnetotransport, and (ii) the semiclassical situation, for which a large number of Landau levels come into play. The method of Feynman diagrams made it possible to obtain expressions for the components of the electrical conductivity tensor in both limits. In contrast to the simplified case of delta-correlated disorder, taking into account a long-range impurity potential (Coulomb interaction, in particular) introduces a new length scale, which affects significantly the system behavior.We showed that the magnetoresistance can deviate from linear behavior as a function of the magnetic field for a certain class of impurity potentials.

5. Superconducting properties of a doped 3D topological insulator.

In the future, we plan to study superconductivity in the rather complex materials studied in this completed project. In such systems, the superconducting order parameter must have nontrivial symmetry and, possibly, topology. As a first step and gaining experience for solving such problems, we analyzed the superconducting properties of a bulk doped 3D topological insulator (see Ref. 4 below). We have shown that the hexagonal warping of the Fermi surface, associated with the real symmetry of the crystal lattice of such materials, stabilizes the nematic spin-triplet superconducting phase with Eu pairing. The temperature dependence of this order parameter differs from the classical BCS dependence. In particular, the ratio, Δ(0)/Tc, of the order parameter to the critical temperature differs from the BCS ratio. This value depends on the chemical potential (i.e. doping). The connection between the obtained results and experimental observations is discussed.

6. Jump-like unraveling of Markovian open quantum systems.

We introduce jump-time unraveling as a distinct description of dissipative open quantum systems (see Refs. 9 and 10 below). As our starting point, we consider quantum jump trajectories, which emerge, physically, from continuous quantum measurements, or, formally, from the unraveling of Markovian quantum master equations. If the stochastically evolving quantum trajectories are ensemble-averaged at specific times, the resulting quantum states are solutions to the associated quantum master equation. We demonstrate that quantum trajectories can also be ensemble-averaged at specific jump counts. The resulting jump-time-averaged quantum states are then solutions to a discrete, deterministic evolution equation, with time replaced by the jump count. This jump-time evolution represents a trace-preserving quantum dynamical map if and only if the associated open system does not exhibit dark states. However, in the presence of dark states, jump-time-averaged states may decay into the dark states and the jump-time evolution may eventually terminate. Jump-time-averaged quantum states and the associated jump-time evolution are operationally accessible in continuous measurement schemes, when quantum jumps are detected and used to trigger the readout measurements. We illustrate the jump-time evolution with the examples of a two-level system undergoing relaxation or dephasing, a damped harmonic oscillator, and a free particle exposed to collisional decoherence.

The main results of the project were published in the following papers:

1. Sboychakov A. O., Rozhkov A. V., Rakhmanov A. L., Nori Franco. Many-body effects in twisted bilayer graphene at low twist angles. Physical Review B, 2019, 100, no 4, id 045111.
2. Rakhmanov A. L., Kugel K. I., Sboychakov A. O.. Coexistence of Spin Density Wave and Metallic Phases Under Pressure. Journal of Superconductivity and Novel Magnetism, 2020, 33, no 8, 2405.
3. Sboychakov A. O., Rozhkov A. V., Rakhmanov A. L., Nori Franco. Spin density wave and electron nematicity in magic-angle twisted bilayer graphene. Physical Review B, 2020, 102, no 15, id 155142.
4. Akzyanov R. S., Khokhlov D. A., Rakhmanov A. L.. Nematic superconductivity in topological insulators induced by hexagonal warping. Physical Review B, 2020, 102, no 9, id 094511.
5. Sboychakov A. O., Rozhkov A. V., Kugel K. I., Rakhmanov A. L., Phase Separation in a Spin Density Wave State of Twisted Bilayer Graphene, JETP Letters, 2020,112, no 10, 651.
6. Rodionov Ya. I., Kugel K. I., Aronzon B. A., Nori Franco. Effect of disorder on the transverse magnetoresistance of Weyl semimetals. Physical Review B, 2020, 102, no 20, id 205105.
7. Khokhlov D. A., Rakhmanov A. L., Rozhkov A. V., Sboychakov A. O.. Dynamical spin susceptibility of a spin-valley half-metal. Physical Review B, 2020, 101, no 23, id 235141.
8. Kokanova S. V., Maksimov P. A., Rozhkov A. V., and Sboychakov A. O.. Competition of spatially inhomogeneous phases in systems with nesting-driven spin-density wave state, Physical Review B, 2021, 104, no 7, id 075110.
9. Gneiting C., Rozhkov A. V., and Nori Franco. Jump-time unraveling of Markovian open quantum systems, Physical Review A, 2021, 104, no 6, id 062212.
10. Gneiting C., Koottandavida A., Rozhkov A.V., and Nori F., Unraveling the topology of dissipative quantum systems. Published online: https://arxiv.org/abs/2007.05960 [arXiv]. To appear in Physical Review Research.

(3)相手国との交流（両国の研究者が協力して学術交流することによって得られた成果）

The fruitful collaboration was established due to mutual visits of the members of both teams' members in RIKEN and ITAE during past 17 years. In 2020 and 2021 it was continued on-line. The work on the project was performed in close collaboration, scientific discussions, and ideas exchange between Japan and

Russian researchers. The tasks 1.1, 1.2, 4, and 6 were solved in a particular close cooperation. The results were presented in five collaborative papers (plus other preprints in preparation):

1. Sboychakov A. O., Rozhkov A. V., Rakhmanov A. L., Nori F. Many-body effects in twisted bilayer graphene at low twist angles. Physical Review B, 2019, 100, no 4, id 045111.
2. Sboychakov A. O., Rozhkov A. V., Rakhmanov A. L., Nori F. Spin density wave and electron nematicity in magic-angle twisted bilayer graphene. Physical Review B, 2020, 102, no 15, id 155142.
3. Rodionov Ya. I., Kugel K. I., Aronzon B. A., Nori F. Effect of disorder on the transverse magnetoresistance of Weyl semimetals. Physical Review B, 2020, 102, no 20, id 205105.
4. Gneiting C., Rozhkov A. V., and Nori F. Jump-time unraveling of Markovian open quantum systems, Physical Review A, 2021, 104, no 6, id 062212.
5. Gneiting C., Koottandavida A., Rozhkov A.V., and Nori F., Unraveling the topology of dissipative quantum systems. Published online: https://arxiv.org/abs/2007.05960 [arXiv]. To appear in Physical Review Research.
6. N. Yoshioka, W. Mizukami, F. Nori, “Solving quasiparticle band spectra of real solids using neural-network quantum states”, Communications Physics 4, 106, 2021,
7. Y. Nomura, N. Yoshioka, F. Nori, “Purifying Deep Boltzmann Machines for Thermal Quantum States”, Phys. Rev. Lett. 127, 060601, 2021.
8. Mazanov, Maxim ; Sugic, Danica ; Alonso, Miguel A. ; Nori, Franco ; Konstantin Y. Bliokh.“ Transverse shifts and time delays of spatiotemporal vortex pulses reflected and refracted at a planar interface” Nanophotonics Volume11 Issue 4.
9. Ye-Hong Chen ,Wei Qin ,Roberto Stassi ,Xin Wang ,Franco Nori, “ Fast binomial-code holonomic quantum computation with ultrastrong light-matter coupling” PHYSICAL REVIEW RESEARCH 3, 033275 (2021).
10. Boxi Li, Shahnawaz Ahmed, Sidhant Saraogi, Neill Lambert, Franco Nori, Alexander Pitchford, Nathan Shammah, “Pulse-level noisy quantum circuits with QuTiP” 2022-01-24, volume 6, page 630.
11. Tao Liu, James Jun He, Zhongmin Yang, and Franco Nori, “Higher-Order Weyl-Exceptional-Ring Semimetals” Phys. Rev. Lett. 127, 196801.
12. Clemens Gneiting, Alexander Rozhkov, Franco Nori, "Jumptime unraveling of Markovian open quantum systems", Physical Review A, 2021, 104, no 6, id 062212.

(4)社会的貢献（社会の基盤となる文化の継承と発展、社会生活の質の改善、現代的諸問題の克服と解決に資する等の社会的貢献はどのようにあったか）

The project has a positive effect on society. First and foremost, top-quality research benefits all. The mutually beneficial research collaboration between the RIKEN and Moscow teams is fostering good links and a better understanding between scientists working in both Russia and Japan. These bilateral cooperations are desirable to improve relations between various countries. These are even more important now, after two years of covid-imposed travel bans, where social and scientific isolation has grown to extreme levels.

(5)若手研究者養成への貢献（若手研究者養成への取り組み、成果）

Two PhD students, Khokhlov D. A and Kokanova S. V., participated in the project. For them, it was an important experience of the work within international team of experienced scientists. They significantly improved their scientific level. The obtained results and publications will serve as a basis for their PhD dissertations. One student in Riken (A. Koottandavida) and two Riken postdocs (Clemens Gneiting and Zhou Li) greatly benefitted from these collaborations, leading to several publications (including some preprints to be submitted soon). Other scientists in both sides interacted with both teams, informing and enriching other points of view of several teams. These discussions were fruitful and led to publications in very good physics journals.

(6)将来発展可能性（本研究交流事業を実施したことにより、今後どの様な発展の可能性が認められるか）

The first goal of fundamental research is to solve important open problems in basic science. These solutions must be evaluated by referees from the top physics journals. The two teams, working together, have done this dozens of times in the past. Interesting results in basic science can evolve into future applications in new technologies, such as the development of new materials for various areas, including electronics, spintronics, quantum memory devices, among others. The results of this project will be the basis for future research; in particular, in the study of exotic superconductivity in these important materials and further research of a new type of half-metal.

(7)その他（上記(2)～(6)以外に得られた成果があれば記述してください）
例：大学間協定の締結、他事業への展開、受賞、産業財産権の出願・取得など

Regarding research awards, the Riken-based PI has been listed as a Clarivate "Highly Cited Researcher” in Physics, for 2017, 2018, 2019, 2020 and 2021 (less than 0.1% of physicist are selected). This is the only case in history for a non-Japanese physicist, for work done in Japan. Several of these highly cited papers were done as part of this RIKEN-Russia collaboration. Our research papers are having an impact in research.

The Riken-based PI has also published more than 30 papers in collaboration with Japanese industry (NEC, Hitachi, Toshiba, and NTT), and is now closely working in a five-year collaboration with researchers at NTT. This proves that Japanese industry has found it useful to interact with the Riken-based research group. This very high level of research cooperation between Japanese industry and a non-Japanese theoretical physicist, is extremely rare, if not unprecedented.