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Topological Phases of Ultracold Atoms Beyond Standard Optical Lattices

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14. ABSTRACT
Significant experimental developments in ultracold gases, such as novel optical lattice geometries and dynamic driving, provide unprecedented opportunities to advance our understanding of many-body physics. Motivated by these developments, the proposed research carries out systematic theoretical studies on three emergent topics, each of which contains exciting unique aspects of no prior analogue in solids. The first topic is correlated and topological phases of interacting atoms on the higher orbital bands of optical lattices with non-standard geometry. The proposed research will investigate the inter-band pairing of polarized fermions, topological chiral p-wave superfluids from s-wave interaction, and correlated orbital phases by repulsive interaction. The second topic explores the topological superfluid and insulating phases of atoms in periodically driven (for instance, shaken or kicked) optical lattices. Quantitative theories will be developed to obtain the phase diagrams and experimental signatures. The third is a longer term goal, proposed to investigate a few fundamental issues in quantum dynamics including time generalization of topological invariants and whether it is quantum mechanically possible to have edge states on the time-space boundary.

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Section 2: Technical Report

Contract/Grant Title: Topological Phases of Ultracold Atoms Beyond Standard Optical Lattices
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2.1 Accomplishments

2.1.1 Research Objectives

The overall goal of this proposal is to discover novel quantum phases of interacting atoms on static optical lattices of non-standard geometry as well as time-periodically modulated optical lattices. Experiments on cold atoms have in recent years opened up new regimes of many-body physics beyond the paradigm of single-band Hamiltonians in stationary optical lattices. This proposal focuses on three emerging topics: (A) topological and other novel states of interacting atoms on higher orbital bands, (B) topological phenomena in periodically driven optical lattices, and (C) emerging fundamental concepts in dynamical quantum systems. The three topics are arranged in the perspective of recent, present and near future optical lattice experiments, for a five-year long term plan. The interest and challenge of the topics are illustrated by examples.

The technical objectives are to develop analytic and numerical methods as well as conceptual innovations to study quantitatively many-body systems in previously inaccessible regimes, and to guide and compare with future closely-related experiments.

The first topic (A) aims at studying multi-orbital interaction effects, particularly interaction driven topological phases, of cold atoms in the higher orbital bands of optical lattices.

The second topic (B) aims at exploring the rich and unique topological phenomena of cold atoms in periodically driven (shaken or kicked) optical lattices.

The third topic (C) is a longer-term objective of investigating a few emerging fundamental concepts regarding the dynamics of quantum many-body systems in general.

2.1.2 Details of accomplishments

This project has achieved the main goals set in the original proposal. The theoretical research supported by this grant focused on discovering novel topological phases and dynamics of ultracold atoms confined in optical lattices. It has led to a series of discoveries such as the atomic chiral orbital superfluid with topological excitations, spontaneous formation of polar superfluid droplets in a *p*-wave interacting Bose gas, *s*+*d*-wave symmetric fermion pairing in a shaking lattice, spin liquid in dipolar magnets, *f*-wave superfluid in repulsively interacting Rydberg Fermi gases, and new collective excitations in a cold gas of bosonic atoms and molecules with *d*-wave interactions (Topic A); topological invariants for quench dynamics, higher-order Floquet topological insulator, and point-gap Weyl semimetal (Topic B); and clean Floquet time crystal, self-ordered time crystal from quasi-periodic driving, and imaginary time crystal (Topic C).

Highlights of major accomplishments:

1. *Novel phases of cold atoms on higher orbital bands: fermions*. The research team discovered that fermionic atoms in circularly shaken square lattice with near resonance frequencies, i.e., tuned close to the energy gap between *s*-band and the *p*-bands, spontaneously pair and condense to form a superfluid of *s*+*d*-wave symmetry [12], due to dynamic orbital mixing. This state is not topological, but novel in its own right with respect to the nontrivial orbital symmetry. This work constitutes the first step towards achieving topological superfluids via lattice shaking, and points to promising shaking proposals for complex Cooper pair order parameter.

Parallel research was carried out to realize topological superfluidity by control of novel lattice geometry. The team put forward a physical scheme to engineer Cooper pairing between even (s-wave) and odd (p-wave) orbital bands in a spin-independent bond-centered square optical lattice. The resultant state is found to be classified by non-trivial topological invariant (C=2) with Majorana fermionic quasi-particle excitations as edge zero modes. The lattice system is closely related to the bipartite checkboard optical lattice configuration realized experimentally by Hamburg group led by A. Hemmerich, albeit their experiments have been mostly focused on bosons until this year.

2. *Novel phases of cold atoms on higher orbital bands: bosons*. Two major results are obtained for bosonic atoms. First, the research team discovered Dirac bosons with π Berry flux [2] in the excitation spectrum in a staggered $p_x \pm ip_y$ Bose-Einstein condensate as observed in the experiment of orbital checkerboard optical lattice at Hamburg. Furthermore, it was found that adding a population imbalance between the p_x+ip_y and p_x-ip_y condensate components opens up a gap at the Dirac point in the spectrum, leading to a finite Chern number as topological invariant and topologically protected edge modes. A detailed description is given on how to implement this proposal experimentally in the Hamburg lab. The experiment is being planned. We expect the theory-experiment collaboration carries on into the next grant period.

Second, going beyond the checkerboard lattice, the research team went on to a qualitatively different class of symmetry and investigated models of superposed *s*- and *p*-orbital bands in hexagonal optical lattices, jointly with an experiment team. The collaborative work has led to the discovery of a chiral atomic superfluid that is proved topological [32]. The time-reversal symmetry breaking was directly observed in the Bose-Einstein condensate through time-of-flight imaging. The fundamental difference from fermionic case is that the topologically protected edge states are not at zero energy, as opposed to what would be typically tied to Fermi level for the latter. This opens up the exciting opportunity to probe and manipulate topological bosonic superfluid.

3. *Novel dynamic phases of quantum matter: clean Floquet time crystal [13] and imaginary time "temperature" crystal [23].* First, our team found a counter example to show in principle that clean Floquet time crystals [13] can generally exist without the need of many-body localization or disorder. Time crystal has been an intriguing subject for systems far away from equilibrium. Recent experiments found such a phase both in the presence and absence of localization, while in theories localization by disorder is usually assumed a priori. To the best of our knowledge, this work is the first counter example in theory that changes the previously assumed understanding on the condition for time crystal. Robust time crystalline orders are found in the strongly interacting regime along with the emergent integrals of motion in the dynamical system, being characterized by level statistics and the out-of-time-ordered correlators. Two cold atom experimental schemes were introduced to realize such "clean" Floquet time crystals, one by making use of dipolar gases and another by synthetic dimensions.

Second, the research team introduced the concept of imaginary time crystal for thermal open systems [23]. Temperature is a fundamental thermodynamic variable for matter. Physical observables are often found to either increase or decrease with it, or show a non-monotonic dependence with peaks signaling underlying phase transitions or anomalies. Statistical field theory has established connection between temperature and time: a quantum ensemble with inverse temperature $\beta = 1/k_B T$ (k_B Boltzmann constant) is formally equivalent to a dynamic system evolving along an imaginary time from 0 to iβ in the space one dimension higher. Using a concrete model of hard-core bosons on a lattice interacting with a thermal bath, the research team demonstrated---by Quantum Monte Carlo simulation and field theoretical analysis---an unexpected temperature-periodic oscillation of its macroscopic observables. Its microscopic mechanism is the crystalline order along the imaginary time axis (bounded by inverse temperature *1/T*). Such a temperature crystal generalizes the concept of purely spatial density-wave order by mapping the time axis for Euclidean action to an extra space dimension for free energy.

4. *Numerical many-body techniques for interacting Fermi gases and interacting spins*. The research team has significantly improved the numerical capacity to compute and predict the phases diagrams of interacting Fermi gases and quantum spin models along two lines: the Functional Renormalization Group (FRG) and Tensor Network (TN). We developed FRG for continuum Fermi gases in 2D, and obtained the comprehensive phase diagrams for dipolar Fermi gases [6] and Rydberg-dressed Fermi gases [26]. We further generalized FRG to interacting spin systems, predicting a robust spin liquid phase for dipolar Heisenberg model on the triangular lattice [14]. We also solved the dipolar Heisenberg model, inspired by polar molecule experiments at JILA, on the square lattice using TN [11] and FRG [15] to reveal a quantum paramagnetic region. We have upgraded the FRG algorithm to take advantage of the parallel processing offered by Graphics Processing Units. As a result, the number of running couplings increased from a few hundred thousand, typical of earlier works in the literature, to over 50 million.

5. *Topological properties of quantum dynamics*. We established a theoretical framework to construct the topological invariants for the quench dynamics of band insulators [29] and applied it to characterize the quench dynamics of Chern, quantum spin Hall, and Hopf insulators [30]. We systematically investigated the Floquet phases in periodically driven Chern insulators [7] and *p*-wave superconductors [8,20,31], proposed a versatile scheme to engineer Floquet higher-order topological insulators by multi-step driving of trivial Hamiltonians, and constructed the dynamical topological invariants that accurately predict the appearance of dynamical corner modes [27,28]. We also developed a knot theory to classify non-Hermitian band structures in one dimension [39] and predicted two unique dynamical signatures of non-Hermitian Weyl semimetals in three dimensions [40].

Publications stemming from the research effort:

1. X. Li and W. V. Liu. Physics of higher orbital bands in optical lattices: a review. Reports on Progress in Physics, 79:116401, 2016.
2. Z.-F. Xu, L. You, A. Hemmerich, and W. V. Liu. π-flux Dirac bosons and topological edge excitations in a bosonic chiral p-wave superfluid. Phys. Rev. Lett., 117:085301, 2016.
3. B. Liu, X. Li, R. G. Hulet, and W. V. Liu. Detecting π-phase superfluids with p-wave symmetry in a quasi-one-dimensional optical lattice. Phys. Rev. A, 94:031602, 2016.
4. B. Liu, X. Li, and W. V. Liu. Topological phases via engineered orbital hybridization in noncentrosymmetric optical lattices. Phys. Rev. A, 93:033643, 2016.
5. X.-J. Liu, Z.-X. Liu, K. T. Law, W. V. Liu, and T. K. Ng. Chiral topological orders in an optical Raman lattice. New Journal of Physics, 18:035004, 2016.
6. A. Keles and E. Zhao. Competing many-body instabilities in two-dimensional dipolar Fermi gases. Phys. Rev. A, 94:033616, 2016.
7. I. Satija and E. Zhao. Cosine edge modes in a periodically driven quantum system. Phys. Rev. B, 94:245128, 2016.
8. E. Zhao. Anatomy of a periodically driven p-wave superconductor. Zeitschrift für Naturforschung A, 71:883, 2016.
9. H. Zou, B. Liu, E. Zhao, and W. V. Liu. A continuum of compass spin models on the honeycomb lattice. New Journal of Physics, 18:053040, 2016.
10. Z.-F. Xu, A. Hemmerich, and W. V. Liu. Odd-parity topological superfluidity for fermions in a bond-centered square optical lattice. Phys. Rev. A, 96:053607, 2017.
11. H. Zou, E. Zhao, and W. V. Liu. Frustrated magnetism of dipolar molecules on a square optical lattice: Prediction of a quantum paramagnetic ground state. Phys. Rev. Lett., 119:050401, 2017.
12. A. Keles, E. Zhao, and W. V. Liu. Effective theory of interacting fermions in shaken square optical lattices. Phys. Rev. A, 95:063619, 2017.
13. B. Huang, Y.-H. Wu, and W. V. Liu. Clean Floquet time crystals: Models and realizations in cold atoms. Phys. Rev. Lett., 120:110603, 2018.

14. A. Keles and E. Zhao. Absence of long-range order in a triangular spin system with dipolar interactions. Phys. Rev. Lett., 120:187202, 2018.
15. A. Keles and E. Zhao. Renormalization group analysis of dipolar Heisenberg model on square lattice. Phys. Rev. B, 97:245105, 2018.
16. E. Zhao. Topological circuits of inductors and capacitors. Annals of Physics, 399:289–313, 2018.
17. Z. Li, J.-S. Pan, and W. V. Liu. Spontaneous formation of polar superfluid droplets in a p-wave interacting Bose gas. Phys. Rev. A, 100:053620, 2019.
18. B. Huang and W. V. Liu. Moiré localization in two-dimensional quasiperiodic systems. Phys. Rev. B, 100:144202, 2019.
19. H. Zou, E. Zhao, X.-W. Guan, and W. V. Liu. Exactly solvable points and symmetry protected topological phases of quantum spins on a zig-zag lattice. Phys. Rev. Lett., 122:180401, 2019.
20. H. Hu, I. I. Satija, and E. Zhao. Chiral and counter-propagating Majorana fermions in a p-wave superconductor. New Journal of Physics, 21:123014, 2019.
21. A. Keles, E. Zhao, and W. V. Liu. Scrambling dynamics and many-body chaos in a random dipolar spin model. Phys. Rev. A, 99:053620, 2019.
22. J.-S. Pan, W. V. Liu, and X.-J. Liu. Emergence of the unconventional type-II Nambu- Goldstone modes with topological origin in Bose superfluids. Phys. Rev. Lett., 125:260402, 2020.
23. Z. Cai, Y. Huang, and W. V. Liu. Imaginary time crystal of thermal quantum matter. Chinese Physics Letters, 37(5):050503, 2020.
24. Z. Li, S. Choudhury, and W. V. Liu. Fast scrambling without appealing to holographic duality. Phys. Rev. Research, 2:043399, 2020.
25. Z. Li, J.-S. Pan, and W. V. Liu. Superfluid phases and excitations in a cold gas of d-wave interacting bosonic atoms and molecules. arXiv:2001.04331, 2020.
26. A. Keles, E. Zhao, and X. Li. F-wave superfluidity from repulsive interaction in Rydberg-dressed Fermi gas. Phys. Rev. A, 101:023624, 2020.
27. B. Huang and W. V. Liu. Floquet higher-order topological insulators with anomalous dynamical polarization. Phys. Rev. Lett., 124:216601, 2020.
28. H. Hu, B. Huang, E. Zhao, and W. V. Liu. Dynamical singularities of Floquet higher-order topological insulators. Phys. Rev. Lett., 124:057001, 2020.
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30. H. Hu, C. Yang, and E. Zhao. Quench dynamics of Hopf insulators. Phys. Rev. B, 101:155131, 2020.
31. H. Hu, E. Zhao, and I. I. Satija. Tuning the topology of p-wave superconductivity in an analytically solvable two-band model. Phys. Rev. B, 102:235156, 2020.
32. X.-Q. Wang, G.-Q. Luo, J.-Y. Liu, W. V. Liu, A. Hemmerich, and Z.-F. Xu. Evidence for an atomic chiral superfluid with topological excitations. Nature, 596:227–231, 2021.
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36. M. Arzamasovs, S. Li, W. V. Liu, and B. Liu. Topological semimetal and superfluid of s-wave interacting fermionic atoms in an orbital optical lattice. arXiv:2101.03774, 2021.
37. S. Choudhury and W. V. Liu. Self-ordered time crystals: Periodic temporal order under quasiperiodic driving. arXiv:2109.05318, 2021.
38. W. V. Liu. Breach pair superfluidity: a brief review. arXiv:2109.02208, 2021. To appear in Festschrift Volume in Honor of Frank Wilczek, World Scientific.
39. H. Hu and E. Zhao. Knots and non-Hermitian Bloch bands. Phys. Rev. Lett., 126:010401, 2021.
40. H. Hu, E. Zhao, and W. V. Liu. Dynamical signatures of point-gap Weyl semimetal. arXiv:2107.02135, 2021.
41. Bartlett, H. Hu, and E. Zhao. Illuminating the bulk-boundary correspondence of a non-Hermitian stub lattice with Majorana stars. Phys. Rev. B 104, 195131.
42. H. Wang, S. Li, M. Arzamasovs, W. V. Liu, B. Liu. Manipulating Goldstone modes via the superradiant light in a bosonic lattice gas inside a cavity. arXiv:2110.02434, 2021

2.1.3 How were the results disseminated

New results obtained from this project were timely posted to the standard preprint server arxiv.org and then submitted to peer-reviewed academic journals such as Nature, Physical Review Letters, Physical Review A and the like for final publication. Results were also exchanged and delivered through research seminars, colloquia, and conference talks to the physics community, both nationally and internationally.

The project has produced over 40 papers published in peer reviewed journals or currently under peer review, including 13 in Physical Review Letters, one in Nature, and one review article in Reports on Progress in Physics.

2.2 Impacts

The theoretical research supported by this grant has achieved the main goal of discovering and understanding novel topological phases and dynamics of ultracold atoms confined in optical lattices. It has produced over 40 papers published in peer reviewed journals or under peer review, including 13 in Physical Review Letters, one in Nature, and one review article in Reports on Progress in Physics.

(1) The project directly impacts the field of cold atoms. Each proposed topic started from concrete theoretical models, completed by systematic analytical and numerical analysis, and concluded with falsifiable predictions for experimental comparison. The theoretical thrusts supported by this grant have already led to experimental verification in the relatively short time frame of the grant life, for example, the observation of chiral atomic

superfluid with topological excitations. It is expected to stimulate or guide more near-future experiments.

Examples of direct impact to experimental programs:

A) Collaboration with Rice University/R. Hulet group:
   - B. Liu, X. Li, R. G. Hulet, and W. V. Liu. Detecting π-phase superfluids with p-wave symmetry in a quasi-one-dimensional optical lattice. Phys. Rev. A, 94:031602, 2016.

B) University of Hamburg/A. Hemmerich group: Through the life of this grant, the Hamburg experimental group leader (Prof. Hemmerich) has been in regular communication on orbital physics with one of PIs (Liu). Three joint articles (1 PRL, 1 PRA, 1 Nature) on this topic have been published. One of the outcomes, for example, is a joint theory-experiment research on bosons, reported in Section 2.1.2, Item 2 “higher orbital bosons”.

   In addition, the Hamburg group has made significant progress with fermionic atoms. In 2021, they reported their first ever “fermion” experiment in higher orbital bands:
   - M. Hachmann, Y. Kiefer, J. Riebesehl, R. Eichberger, A. Hemmerich. Quantum degenerate Fermi gas in an orbital optical lattice. Phys. Rev. Lett. 127, 033201 (2021)

   It is evident that the theoretical ideas on orbital physics presented in the proposal served well as part of major motivation and guidance for the Hamburg fermion experiment. Their experimental breakthrough is many years in planning, and their paper cited our theoretical work, in particular [1] as key motivation.

(2) The insights gained through this project on interacting quantum gases in dynamical optical lattices contribute to the toolbox to realize novel quantum phases of matter in and out of equilibrium, an active research frontier involving several subfields of physics beyond the context of dynamical optical lattices. While optical lattice is one of the major quantum simulation platforms available, the models and results found in this project regarding dynamical quantum many-body effects are also relevant to coupled superconducting qubits, trapped ion arrays, open photonic systems, and other related artificial quantum many-body systems. For example, the theoretical framework classifying and characterizing higher order Floquet topological phases, quench dynamics of band insulator, and non-Hermitian band structure are general. It extends the topological classification based on symmetry from equilibrium to dynamical quantum states of matter, from closed systems to open non-Hermitian models.

(3) The numerical many-body algorithms developed and improved, including Functional Renormalization Group and Tensor Network ansatz, can be applied to other interacting quantum many-body systems such as correlated electronic materials or quantum magnets.

2.3 Changes

Changes in approach
None

Problems or delays
None

Expenditure Impacts
No change

Significant changes in the use or care of human subjects, vertebrate animals and/or biohazards
None

2.4 Technical Updates

This section will include any and all technical updates that you would like to provide to your program officer. You are encouraged to upload graphs and other visualizations that highlight the work done during this reporting period. Program Officers may request additional information that is specific to your research topics.

Selected technical results: Our theoretical prediction of atomic chiral topological superfluid led to experimental discovery.

Nature 596, 227-231(2021), [https://www.nature.com/articles/s41586-021-03702-0], by one of PIs (Liu) and experimental collaborators.

A cold gas of Rb-87 atoms was populated into the superposition of s and p orbitals in a boron nitride hexagonal optical lattice (Fig 1 below). It undergoes Bose-Einstein condensation and spontaneously formation of global angular momentum. The state breaks the time reversal symmetry, manifest through the asymmetry in $k \rightarrow -k$ transformation in the momentum distribution of atoms (bottom row of Fig 2). See the original article for full details.

Fig 1

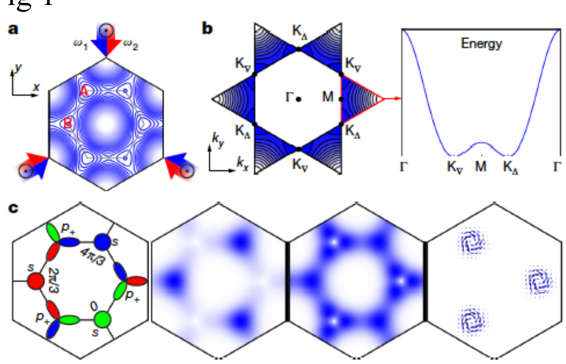

Fig 2