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Final Technical Report

OSTI: 2537889 DE-SC0022106 Magnetism in Moiré Materials

PERFORMANCE PERIOD: 09/01/2021-07/31/2023
AWARDEE NAME: UNIVERSITY OF TEXAS AT AUSTIN
PRINCIPLE INVESTIGATOR: ALLAN H. MACDONALD

Final Technical Report for Award #: DE-SC0022106
Magnetism in Moiré Materials

This grant supported theoretical condensed matter physics research related mainly to magnetism in moiré materials. The moiré materials platform idea was developed mainly by this PI and mainly with DOE-BES support. Because it can create artificial crystals with lattice constants on the 10 nm scale, it is a flexible platform for strong correlations. Because of band crossings in the host materials and a tunable interplay between interlayer tunneling and potential differences between layers it is a flexible platform for tunable topological matter. This award supported early research on magnetism in moiré materials, which is unusual because magnetism often occurs directly in orbital degrees of freedom – instead of being created in spin and induced in orbital degrees of freedom by spin-orbit coupling. Orbital magnetism results in integer and fractional quantum anomalous Hall effects and electrically tunable magnetization reversal - among other phenomena.

A complete list of publications that were supported by this grant, listed in reverse chronological order, is appended below. All publications related to work supported by this grant have now been published – except for preprint 12 which we may leave as a preprint and follow up later in a different form.

Publications 1,3, and 17 are related to orbital magnetism and integer and fractional quantum anomalous Hall effects in moiré materials. This is one of the most unique aspects of the interaction physics that has been discovered in moiré materials. I view publication 1 as an important contribution that identifies the physical mechanism for the fractional quantum anomalous Hall State discovered in twisted MoTe_2 . I hope that publication 3 will stand the test of time as a valuable review of the quantum anomalous Hall effect and orbital magnetism.

Publications 2, 7, and 11 relate to generalized magnetic fluctuations in moiré materials as a mechanism for superconductivity. Superconductivity has shown itself to be common in the phase diagrams of most moiré materials. The ability to tune the number of electrons per effective atom electrically is an important advantage of moiré materials. The consistent proximity of magnetic and superconducting states in phase diagrams make it clear that magnetic fluctuations mechanisms are active. I expect that the moiré material platform will prove very valuable in advancing understanding of superconductivity in atomic scale materials like cuprates.

Publications 4, and 14 related to density-wave states, for example Wigner crystals, in moiré materials. Density-wave insulators are also common in the phase diagrams of moiré materials, and compete with fractional Chern insulators. Advancing understanding of the competition between these two different types of insulators has been a major theme of research undertaking under this grant.

Some other topics that arose during this research resulted in publications – including interfaces between two-dimensional magnetic insulators and graphene (Publications 5 and 6), weak localization (Publication 9) as a probe of intervalley order, itinerant electron magnetism (Publication 8), and phonon Hall effects (Publication 12).

Workforce Training:

This grant financially supported the education and career development of graduate students Igor Blinov and Naichao Hu and postdoctoral researcher Wei Qin. Hu and Blinov completed their Ph.D s. during the summer 2023 semester. Hu is now a postdoctoral researcher at the University of Leuven in Belgium and Blinov is a postdoctoral researcher in Russia. Qin is a faculty member at the University of Science and Technology of China. Some other students (Nicolas Morales-Duran, Jingtian Shi, Nemin Wei, Yong Zeng) were indirectly supported by this project, while receiving primary financial support from teaching assistantships or other related grants. Morales-Duran is a postdoc at the Flatiron Institute in New York, Jingtian Shi at Argonne National Lab, Yong Zeng at Columbia University, and Nemin Wei at Yale University.

PUBLICATIONS THAT ACKNOWLEDGE THIS GRANT:

1. Morales-Durán, N., Wei, N., Shi, J., and MacDonald, A. H., "Magic Angles and Fractional Chern Insulators in Twisted Homobilayer Transition Metal Dichalcogenides," Phys. Rev. Lett. 132 (9), 09662 (March 1, 2024).
2. Qin, W., Zou, B., and MacDonald, A. H., "Critical magnetic fields and electron-pairing in magic-angle twisted bilayer graphene," Phys Rev B 107, 024509 (January 26, 2023).
3. Chang, C.-Z., Liu, C.-X., and MacDonald, A. H., "Colloquium: Quantum anomalous Hall effect," Rev of Mod Phys 95, 011002 (January 23, 2023).
4. Morales-Durán, N., Potasz, P., and MacDonald, A. H., "Magnetism and Quantum Melting in Moiré-Material Wigner Crystals," Phys. Rev. B 107, 235131 (June 14, 2023).
5. Shi, J., and MacDonald, A. H., "Probing the Magnetic State of a Kitaev Material with Graphene," Phys Rev B 108, 064401 (August 1, 2023).

6. Cardoso, C., Costa, A. T., MacDonald, A. H., and Fernández-Rossier, J., "Strong magnetic proximity effect in Van der Waals heterostructures driven by direct hybridization," *Phys. Rev. B* 108, 184423 (November 22, 2023).
7. Qin, W., Huang, C., Wolf, T., Wei, N., Blinov, I., and MacDonald, A. H., "Functional Renormalization Group Study of Superconductivity in Rhombohedral Trilayer Graphene," *Phys. Rev. Lett.* 130 (14) 146001 (April 4, 2023).
8. Potasz, P., Morales-Durán, N., Hu, N. C., and MacDonald, A. H., "Itinerant ferromagnetism in transition metal dichalcogenides moiré superlattices," *Phys. Rev. B* 109, 045144 (January 23, 2024).
9. Wei, N., Zeng, Y., and MacDonald A. H., "Weak localization as a probe of intervalley coherence in graphene multilayers," *Physical Review B* 111 (24), L241103 (2025).
10. Shi, J. and MacDonald, A. H., "Magnetic states of graphene proximitized Kitaev materials," *Physical Review B* 108, 064401 (August 1, 2023).
11. Huang, C., Wei, N., Qin, W., and MacDonald, A. H., "Pseudospin Paramagnons and the Superconducting Dome in Magic Angle Twisted Bilayer Graphene," *Phys Rev Lett* 129 187001 (October 24, 2022).
12. Flebus, B., and MacDonald, A.H., "The phonon Hall viscosity of ionic crystals," *arXiv:2205.13666* (May 26, 2022).
13. Zeng, Y., Wei, N., and MacDonald, A.H., "Layer Pseudospin Magnetism in Transition-Metal-Dichalcogenide Double-Moirés," *Phys. Rev. B* 106 (16) 165106 (October 6, 2022).
14. Kaushal, N., Morales-Durán, N., MacDonald, A. H., and Dagotto, E., "Magnetic ground states of honeycomb lattice Wigner crystals," *Communications Physics* 5, 289 (November 18, 2022).
15. Morales-Durán, N., Hu, N., Potasz, P., and MacDonald A. H., "Nonlocal Interactions in Moiré Hubbard Systems," *Phys Rev Lett* 128, 217202 (May 24, 2022).
16. Lei, C., and MacDonald, A. H., "Simple accurate model of silicon donor arrays," *Phys. Rev. B* 106, 045305, (July 25, 2022).
17. Kuiri, M., Coleman, C., Gao, Z., Vishnuradhan, A., Watanabe, K., Taniguchi, T., Zhu, J., MacDonald, A. H., and Folk, J., "Spontaneous time-reversal symmetry breaking in twisted double bilayer graphene," *Nature Communications* 13 6468 (October 29, 2022).