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Band Engineering New Phases of Matter with Ultracold Atoms

Vito Scarola
VIRGINIA POLYTECHNIC INST AND STATE UNIVERSITY

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14. ABSTRACT
In this three-year effort we have made significant progress in understanding how to engineer novel phases of matter with atoms in optical lattices.
Optical lattices applied to trapped atomic gases offer considerable versatility in engineering quantum states. Recent advances in optical control have
taken exploration of quantum degenerate matter in an exciting new direction: band engineering with synthetic fields. In this context, synthetic fields
act as effective magnetic and/or electric fields on neutral quantum gases. Our work models how novel quantum states derive from engineered bands
because tailored bases emphasize interaction effects. Novel quantum states we studied include: Wigner crystals, emergent Luttinger liquids,
many-body localization, the Bose-Glass, as well as other. Our methods include numerical simulations of models constructed to capture effects in
ongoing experiments. Specific methods include numerical diagonalization, the time evolving block-decimation algorithm, and mean-field theories.
Our work fosters the identification of novel states of matter with ultracold atomic gases derived from band engineering of importance to ongoing
Air Force research efforts to build such experiments.

15. SUBJECT TERMS
band engineering, new phases of matter

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FINAL REPORT: BAND ENGINEERING NEW PHASES OF MATTER WITH ULTRACOLD ATOMS

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Section **Page**

1.0 ABSTRACT

In this three-year effort we have made significant progress in understanding how to engineer novel phases of matter with atoms in optical lattices. Optical lattices applied to trapped atomic gases offer considerable versatility in engineering quantum states. Recent advances in optical control have taken exploration of quantum degenerate matter in an exciting new direction: band engineering with synthetic fields. In this context, synthetic fields act as effective magnetic and/or electric fields on neutral quantum gases. Our work models how novel quantum states derive from engineered bands because tailored bases emphasize interaction effects. Novel quantum states we studied include: Wigner crystals, emergent Luttinger liquids, many-body localization, the Bose-Glass, as well as other. Our methods include numerical simulations of models constructed to capture effects in ongoing experiments. Specific methods include numerical diagonalization, the time evolving block-decimation algorithm, and mean-field theories. Our work fosters the identification of novel states of matter with ultracold atomic gases derived from band engineering of importance to ongoing Air Force research efforts to build such experiments.

2.0 SUMMARY

Experiments with ultracold atoms in optical lattices demonstrate strongly correlated states, including superfluids and Mott insulators. But further progress in realizing novel strongly correlated states has been hindered. For example, strict temperature requirements prevent the realization of antiferromagnetic states via super-exchange. Also, Raman lasers used to implement spin-orbit coupling lead to considerable losses and heating near Feshbach resonances where strong interactions are expected to reveal intriguing strongly correlated states. Nonetheless optical lattices offer very precise control over weakly correlated states, i.e., single-particle band structure. Straightforward extensions of optical lattice technology can be used to engineer different single-particle band structures. Our work proposed experiments designed to use the tunability of band structures to avoid obstacles in realizing novel many-body states with optical lattices.

Novel phases of matter derived from strong interactions are possible, but challenges remain. Increasing lattice depth to favor interactions tightly localizes particles in optical lattice sites. The resulting interactions are purely local and limit possibilities. Proposed methods to extend the range of interaction include: virtual processes, i.e., superexchange; promotion of particles to higher bands; placing dipoles in optical lattices; and others.

The following outlines mathematical and numerical methods we constructed and employed:

Exact Diagonalization: The set of flat band problems we tackled are inherently non-perturbative. To study the low energy physics of interactions in flat bands our primary tool was exact diagonalization and related methods, i.e., Lanczozs and Arnoldi methods. By studying the low energy states of interacting models, we identified lattice models with stable (gapped) ground states. The following formalism is designed to rigorously identify novel states in non-perturbative flat band models:

i) Model the band structure of a flat band lattice
ii) Identify and project into flat bands
iii) Compute the interaction matrix elements
iv) Diagonalize the many-body model to obtain the low energy Hilbert space
v) Compare states of physical model with effective models using overlap, energetics
vi) Identify and compute relevant observables

Variational Wavefunctions and Effective Models: Our group has pioneered a new technique to construct wavefunctions for flat bands. This method allows direct construction of wavefunctions (e.g., Jastrow-correlated BCS states, Jastrow-correlated Fermi liquid states, etc.) in second quantization. Direct evaluation of wavefunction amplitudes is generated by a matrix product formulation.

We also constructed effective models to validate and test our proposed emergent states. In 1D we have constructed an effective extended Hubbard model. Variations on this effective Hubbard model allowed us to explore other densities. Diagonalization for the realistic and effective models will allow direct comparison and rigorous interpretation of the results from exact diagonalization.

Mean Field Methods: Mean field numerical methods were used, which include Gutzwiller variational methods for bosons in optical lattices. This method was extended to tackle dynamics in trapped optical lattice systems.

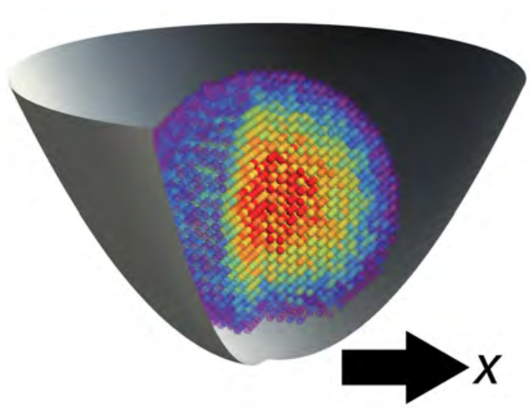
Exact dynamics using Time-Evolving-Blocking-Decimation (TEBD) algorithm: We also used the TEBD algorithm to study exact quantum states and their dynamics in 1D systems. It was generalized to spin-orbit coupled systems to study dynamics of spin flip tunneling.

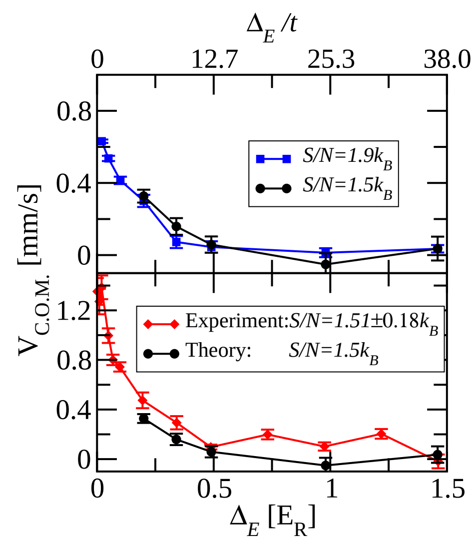
The projects described in this proposal significantly advanced our understanding of atoms in optical lattices. These systems are of direct interest to AFOSR initiatives that are currently under study. The models and simulations guided experiments towards realization of novel states of matter and thereby established new platforms for fundamental science and technological development. The band engineering ideas we discus here have the potential to establish new paradigms in the way we understand the interplay of quantum mechanics and many-body systems.

3.1 TRANSPORT OF HUBBARD-BAND QUASIPARTICLES IN DISORDERED OPTICAL LATTICES

V. W. Scarola and B. DeMarco Phys. Rev. A 92, 053628 (2015) arXiv:1503.07195

Recent experiments use transport of degenerate Fermi gases in optical lattices (Kondov et al. Phys. Rev. Lett. 114, 083002 (2015)) to probe a particularly extreme regime of strong interaction in what can be modeled as an Anderson-Hubbard model. These experiments find evidence for an intriguing insulating phase where quantum diffusion is completely suppressed by strong disorder. Quantitative interpretation of these experiments remains an open problem that requires inclusion of non-zero entropy, strong interaction, and trapping. We argue that the suppression of transport can be thought of as localization of Hubbard-band quasiparticles. We construct a theory of transport of Hubbard-band quasiparticles tailored to trapped optical lattice experiments. We compare the theory directly with center-of- mass transport experiments of Kondov et al. with no fitting parameters. The close agreement between theory and experiments shows that the suppression of transport is only partly due to finite entropy effects. We argue that the complete suppression of transport is consistent with Anderson localization of Hubbard-band quasiparticles. The combination of our theoretical framework and optical lattice experiments offers an important platform for studying localization in isolated many-body quantum systems.





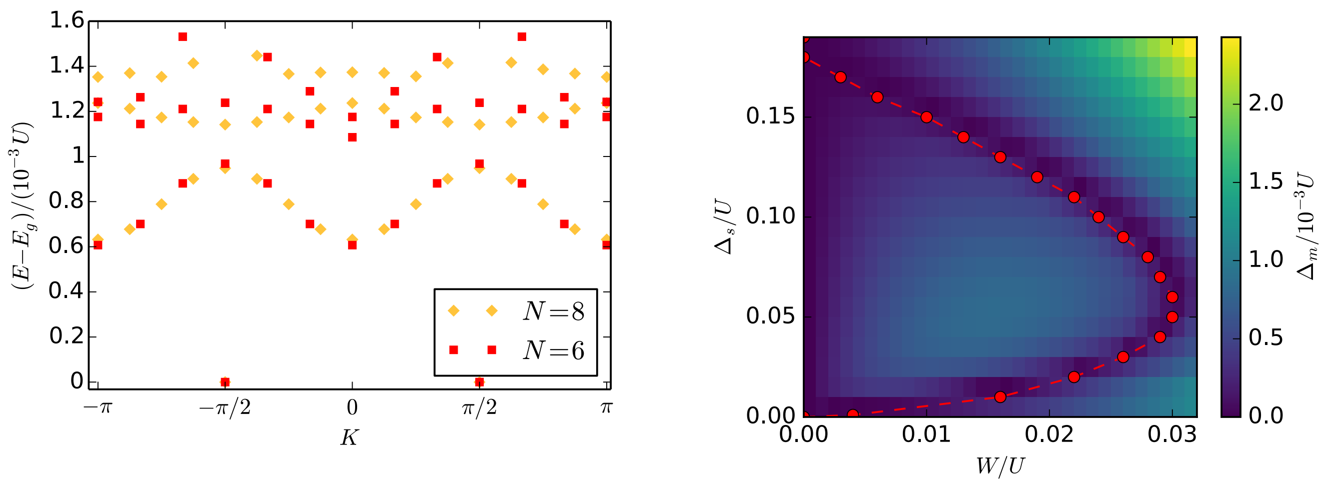
Left: Schematic showing disordered lattice sites in a parabolic trapping potential. The site coloring represents a dense core that gives way to zero density at the edges. The system studied here can be thought of as a strongly interacting high temperature paramagnet with a density less than one at the center.

Top Right: Disorder averaged center-of-mass velocity as a function of the disorder strength for two different entropies. Right Bottom: The circles plot the same as the top panel and the diamonds plot experimental data from DeMarco's group for comparison. The lines are a guide to the eye.

3.2 STABILITY OF EMERGENT KINETICS IN OPTICAL LATTICES WITH ARTIFICIAL SPIN-ORBIT COUPLING

M. Chen and **V.W. Scarola** *Phys. Rev. A* **94,** 43601 (2016).

Artificial spin-orbit coupling in optical lattices can be engineered to tune band structure into extreme regimes where the single-particle band flattens leaving only inter-particle interactions to define many-body states of matter. Lin et al. [Phys. Rev. Lett 112, 110404 (2014)] showed that under such conditions interactions lead to a Wigner crystal of fermionic atoms under approximate conditions: no bandwidth or band mixing. The excitations were shown to possess emergent kinetics with fractionalized charge derived entirely from interactions. In this work we use numerical exact diagonalization to study a more realistic model with non-zero bandwidth and band mixing. We map out the stability phase diagram of the Wigner crystal. We find that emergent properties of the Wigner crystal excitations remain stable for realistic experimental parameters. Our results validate the approximations made by Lin et al. and define parameter regimes where strong interaction effects generate emergent kinetics in optical lattices.

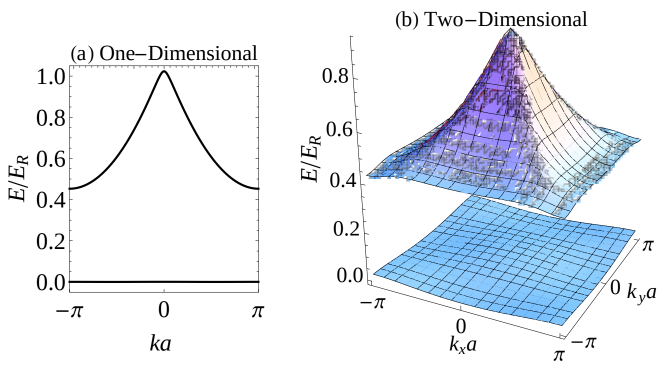


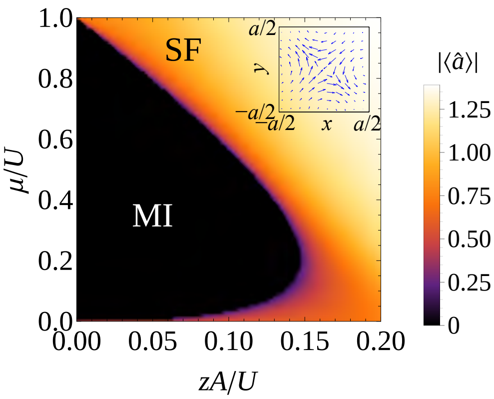
Left: Many-body energies versus total wavevector obtained from diagonalization. The gap shows stability of a Wigner crystal. The dispersive excitation shows emergent kinetics. The data collapse shows that the ground and first excited states are already in the thermodynamic limit. Right: Stability phase diagram of the Wigner crystal with emergent kinetics plotted as function of both the single-particle band gap and the bandwidth. The color coding plots the size of the many-body gap obtained from diagonalization. The circles plot the points where the many-body gap vanishes and the line is a guide to the eye. The Wigner crystal is stable within the lobe. Outside the lobe we have a conventional Luttinger liquid with a gap set by finite-size effects.

3.3 SUPERFLUIDITY IN THE ABSENCE OF KINETICS IN SPIN-ORBIT-COUPLED OPTICAL LATTICES

Hoi-Yin Hui, Y, Zhang, C. Zhang, and **V. W. Scarola** *Phys. Rev. A* **95,** 33603 (2017).

At low temperatures bosons typically condense to minimize their single-particle kinetic energy while interactions stabilize superfluidity. Optical lattices with artificial spin-orbit coupling challenge this paradigm because here kinetic energy can be quenched in an extreme regime where the single-particle band flattens. To probe the fate of superfluidity in the absence of kinetics we construct and numerically solve interaction-only tight-binding models in flat bands. We find that novel superfluid states arise entirely from interactions operating in quenched kinetic energy bands, thus revealing a distinct and unexpected condensation mechanism. Our results have important implications for the identification of quantum condensed phases of ultracold bosons beyond conventional paradigms.





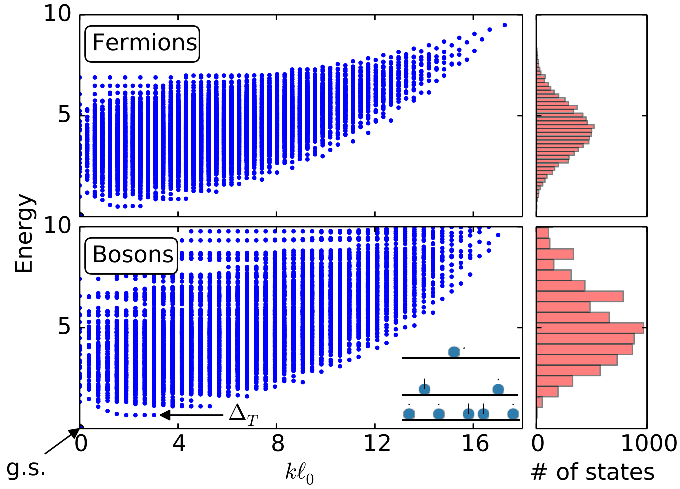
Left: Single particle energy versus wave vector for the lowest two energy bands of (a) the one-dimensional model and (b) the two-dimensional model of spin-orbit coupled atoms in optical lattices. Flat bands are found at low energies.

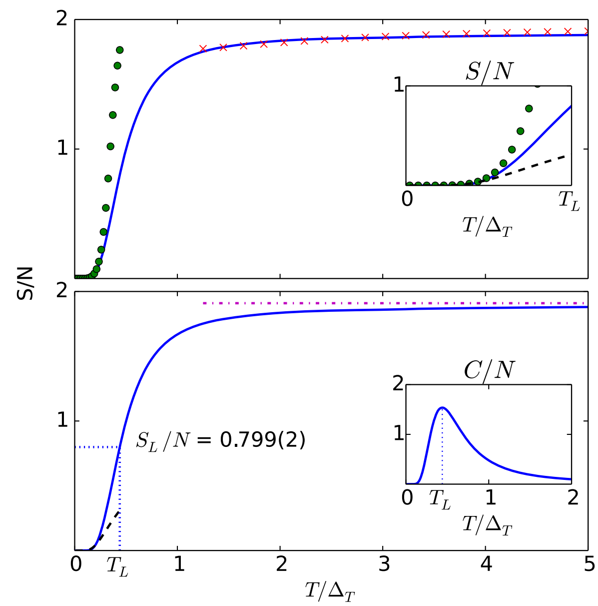
Right: The magnitude of the superfluid order parameter against chemical potential and effective tunneling obtained from mean field theory. The superfluid (SF) and Mott insulator (MI) derive entirely from interactions. The inset shows the spin texture in a unit cell for the 2D system.

3.4 THERMOMETRY FOR LAUGHLIN STATES OF ULTRACOLD ATOMS

P.T. Raum, **V.W. Scarola** Phys. Rev. Lett. 118, 115302 (2017)

Cooling atomic gases into strongly correlated quantum phases requires estimates of the entropy to perform thermometry and establish viability. It is currently unknown how cold chiral spin liquids and other topological phases need to be in order to be realized. The chiral spin liquid maps directly onto Laughlin states of bosons. We construct an ansatz partition function for models of Laughlin states of atomic gases by combining high temperature series expansions with exact diagonalization. Using the ansatz we find that entropies required to observe Laughlin correlations, and therefore chiral spin liquids, with bosonic gases are within reach of current cooling capabilities.





Left: Energy of 8 fermions (bosons) as a function of total wavevector in the lowest Landau level. The ground state is the k=0 Laughlin state set to zero energy. The schematic depicts example excitations. The bosonic Laughlin state can be thought of as one filled level of CFs (bosons attached to one flux quantum). Low energy excitations are CF particle-hole pairs. The histograms show nearly Gaussian state counting.

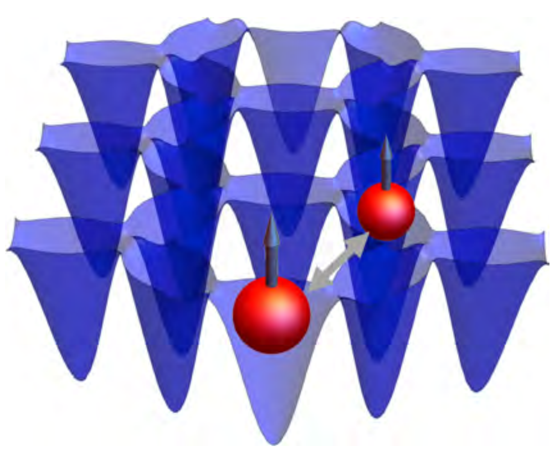
Right: The main panels plot the entropy per particle versus temperature for bosons. The solid lines are obtained from our ansatz. The symbols are other exact results. The agreement between the symbols and the lines shows that the ansatz accurately captures the low and high T limits. The inset plots the heat capacity from the ansatz in the thermodynamic limit. *The number S/N~0.8 indicates the first calculation of the entropy needed to realize a Laughlin state with cold atoms.*

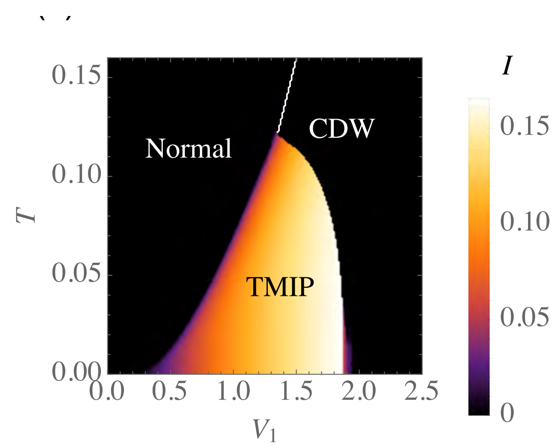
3.5 CHIRAL TOPOLOGICAL PHASES IN OPTICAL LATTICES WITHOUT SYNTHETIC FIELDS

Hoi-Yin Hui, Mengsu Chen, Sumanta Tewari, **V. W. Scarola**

Phys. Rev. A **98,** 023609 (2018). arXiv: 1712.10238

Synthetic fields applied to ultracold quantum gases can realize topological phases that transcend conventional Bose and Fermi-liquid paradigms. Raman laser beams in particular are under scrutiny as a route to create synthetic fields in neutral gases to mimic ordinary magnetic and electric fields acting on charged matter. Yet external laser beams can impose heating and losses that make cooling into many-body topological phases challenging. We propose that atomic or molecular dipoles placed in optical lattices can realize a topological phase without synthetic fields by placing them in certain frustrated lattices. We use numerical modeling on a specific example to show that the interactions between dipolar fermions placed in a kagome optical lattice spontaneously break time-reversal symmetry to lead to a topological Mott insulator, a chiral topological phase generated entirely by interactions. We estimate realistic entropy and trapping parameters to argue that this intriguing phase of matter can be probed with quantum gases using a combination of recently implemented technologies.





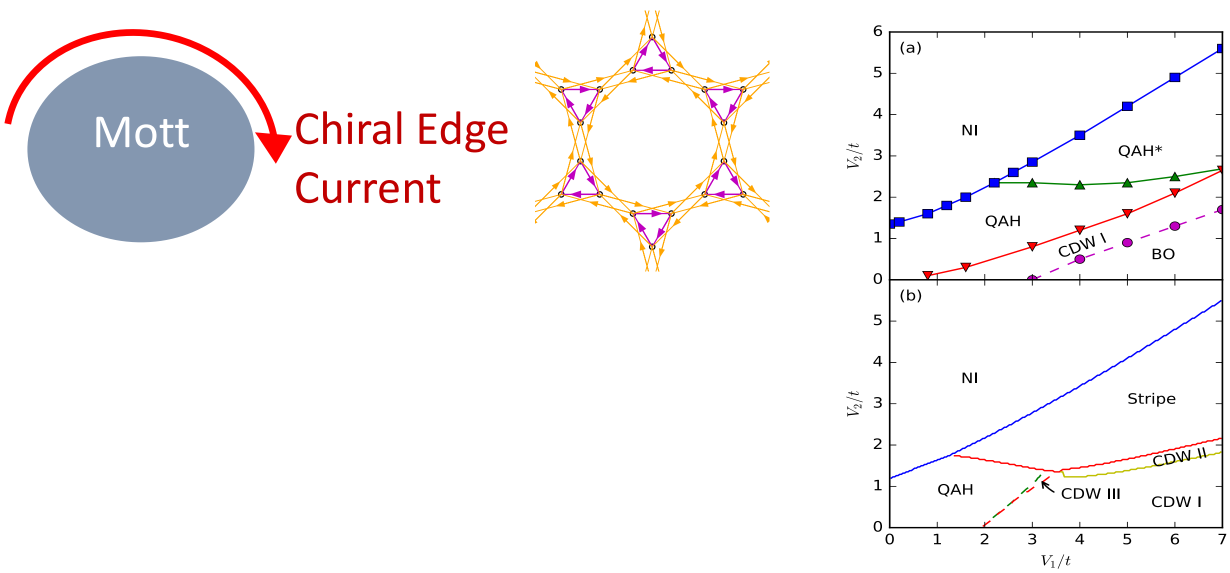
Left: Plot of a kagome optical lattice potential (as implemented in the Stamper-Kurn group) as a function of position in the x-y plane. The two particles represent schematics of dipoles separated in the plane by $|r - r'|$ with moments oriented perpendicular to the plane to ensure mutual repulsion.

Right: The mean-field phase diagram of dipoles in a kagome optical lattice obtained by plotting the magnitude of the current against temperature and interaction strength. The white line uses the density difference between sites, δn, to plot the boundary between the charge density wave ($\delta n > 0$) and the normal phase (an absence of order with $\delta n = 0$). This phase diagram shows that there is a topological phase accessible with dipoles in optical lattices that does not rely on synthetic fields.

3.6 QUANTUM ANOMALOUS HALL STATE FROM SPATIALLY DECAYING INTERACTIONS ON THE DECORATED HONEYCOMB LATTICE

Mengsu Chen, Hoi-Yin Hui, Sumanta Tewari, **V. W. Scarola**
Phys. Rev. B **97,** 035114 (2018). arXiv:1705.05829

Topological phases typically encode topology at the level of the single particle band structure. But a remarkable new class of models shows that chiral quantum anomalous Hall effects can be driven exclusively by interactions, while the parent non-interacting band structure is topologically trivial. Unfortunately, these models have so far relied on interactions that do not spatially decay and are therefore unphysical. We study a model of spinless fermions on a decorated honeycomb lattice. Using complementary methods, mean-field theory and exact diagonalization, we find a robust quantum anomalous Hall phase arising from spatially decaying interactions. Our finding paves the way for observing the quantum anomalous Hall effect driven entirely by interactions.



Left: Schematic of chiral currents circulating a topological Mott insulator.

Center: Chiral bond currents in the quantum anomalous Hall phase computed using exact diagonalization

Right: (a) Phase diagram obtained using exact diagonalization on the decorated honeycomb lattice. The symbols are results from calculations and the lines are a guide to the eye. The chiral quantum anomalous Hall phase arises in the center. (b) The same as (a) but the lines plot transitions obtained from self-consistent mean field theory. The agreement between panels (a) and (b) shows strong evidence for a robust chiral state.

3.7 EQUILIBRATION DYNAMICS OF STRONGLY INTERACTING BOSONS IN 2D LATTICES WITH DISORDER

Mi Yan, Hoi-Yin Hui, Marcos Rigol, **Vito W. Scarola** arXiv:1606.08439
Phys. Rev. Lett. 119, 073002 (2017)

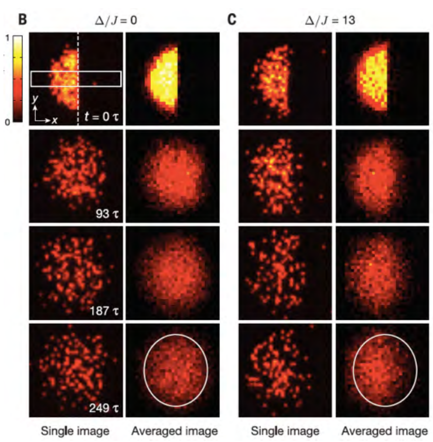
Motivated by recent optical lattice experiments in Immanuel Bloch's group [Choi et al., Science 352, 1547 (2016)], we study the dynamics of strongly interacting bosons in the presence of disorder in two dimensions. We show that Gutzwiller mean-field theory (GMFT) captures the main experimental observations, which are a result of the competition between disorder and interactions. Our findings highlight the difficulty in distinguishing glassy dynamics, which can be captured by GMFT, and many-body localization, which cannot be captured by GMFT, and indicate the need for further experimental studies of this system.

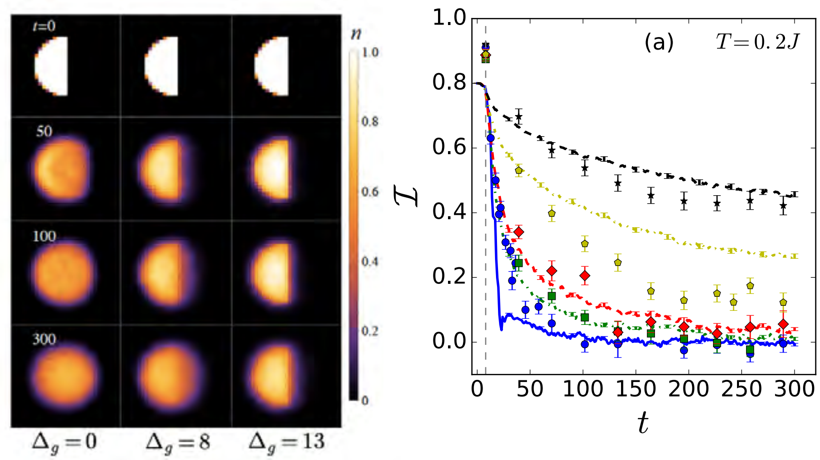
J. Choi, et. al.,

Science '16

M. Yan, H. Hui, M. Rigol, V.W. Scarola

Phys. Rev. Lett. 119, 073002 (2017)





Left: Results from atomic gas microscope experiments in Immanuel Bloch's group. The strong disorder prevents thermalization.

Center: Our theory calculations for the same parameters as experiments in Choi et al.

Right: Imbalance as function of time for both theory (lines) and experiments (symbols). The close comparison shows that mean field theory is a good approximation. The assertion that many-body localization was observed therefore requires further experiments probing the difference between mean field and experiment since mean field theory does not have many-body localization.

APPENDIX A- PRESENTATIONS GIVEN RELATED TO THIS PROJECT

Invited Presentations by PI Scarola and collaborators:
(Group members are underlined and PI is in bold)

2015 (beginning 10/1):

Engineering Strongly Correlated Magnetic States with Ultracold Atoms
SUNY Stoney Brook Stoney Brook, NY
Vito Scarola

Evidence for Topological Stripes Derived from Fractional Chern Insulators Institute for Condensed Matter Theory, University of Illinois Urbana-Champaign
Champaign, Il
Vito Scarola

2016:

Dynamics of Hubbard-Band Quasiparticles in Disordered Optical Lattices
2016 APS March Meeting, MD
Vito Scarola

Strengthening Supersolids with Disorder in the Extended-Bose Hubbard Model
2016 APS March Meeting, MD
F. Lin (presenter) and **Vito Scarola**

Stability of fractional quantum Hall states
Workshop on Innovative Nanoscale Devices and Systems, HI
Vito Scarola

Stability of Fractional Quantum Hall States
California State University Long Beach, CA
Vito Scarola

Dynamics and New States in Optical Lattices
Joint Quantum Institute-University of Maryland, MD
Vito Scarola

2017:

Equilibration Dynamics of Strongly Interacting Bosons in 2D Lattices with Disorder
APS March Meeting, New Orleans, Louisiana
Mi Yan (presenter), Hoi-Yin Hui, Marcos Rigol, **Vito Scarola**

Stability of Emergent Kinetics in Optical Lattices with Artificial Spin-Orbit Coupling
APS March Meeting, New Orleans, Louisiana
Mengsu Chen (presenter) and **Vito Scarola**

Superfluidity in the absence of kinetics in spin-orbit- coupled optical lattices
APS March Meeting, New Orleans, Louisiana
Hoi-Yin Hui (presenter), Yongping Zhang , Chuanwei Zhang, **Vito Scarola**

Thermometry for Laughlin States of Ultracold Atoms
APS March Meeting, New Orleans, Louisiana
Peter Raum (presenter) and **Vito Scarola**

Density Assisted Tunneling of Fermions in Optical Lattices
APS March Meeting, New Orleans, Louisiana
Vito Scarola (presenter), Wenchao Xu, William Morong, Hoi Hui, Brian DeMarco

Topological Mott Insulators in Certain Frustrated Lattices
Workshop on Innovative Nanoscale Devices and Systems Kona, HI
Vito Scarola (presenter), Mengsu Chen, Hoi Hui

2018 (ending 12/28):

Topological phases from dipolar interactions on kagome optical lattices
APS March Meeting, Los Angeles, CA
Hoi-Yin Hui (presenter), Mengsu Chen, Sumanta Tewari, **Vito Scarola**

Topological Mott Insulators in Certain Frustrated Lattices
APS March Meeting, Los Angeles, CA
Vito Scarola (presenter), Mengsu Chen, Hoi-Yin Hui, Sumanta Tewari

Atomic Gas Microscopes: Tools for Quantum Emulation and Prospects for Quantum Information Processing
Oak Ridge National Laboratory, Oak Ridge TN
Vito Scarola

Optical Measurements in the Fractional Quantum Hall Regime
Optoelectronics 2018
Philadelphia, PA
Vito Scarola

APPENDIX B- PUBLICATIONS SUPPORTED BY THIS PROJECT
(PI in bold and group members underlined)

1. Chen, M., Hui, H.-Y., Tewari, S. & **Scarola, V. W**. Quantum anomalous Hall state from spatially decaying interactions on the decorated honeycomb lattice. *Phys. Rev. B* **97,** 035114 (2018).

2. Hui, H.-Y., Chen, M., Tewari, S. & **Scarola, V. W**. Chiral Topological Phases in Optical Lattices Without Synthetic Fields. *Phys. Rev. A* **98,** 23609 (2018).

3. Xu, W., Morong, W., Hui, H.-Y., **Scarola, V. W**. & DeMarco, B. Correlated Spin-Flip Tunneling in a Fermi Lattice Gas. *arxiv:1711.02061* (2017).

4. Yan M, Qian Y, Hui H, Gong M, Zhang C, & **Scarola V**, Spin-orbit-driven transitions between Mott insulators and finite-momentum superfluids of bosons in optical lattices. *Phys. Rev. A* **96,** 053619 (2017).

5. A. J. McCaskey, E. F. Dumitrescu, D. Liakh, M. Chen, W. Feng, T. S. Humble, A Language and Hardware Independent Approach to Quantum-Classical Computing arXiv:1710.01794 (2017).

6. A. McCaskey, E. Dumitrescu, M. Chen, D. Lyakh, T. S. Humble, Validating Quantum-Classical Programming Models with Tensor Network Simulations arXiv:1807.07914 (2018).

7. Yan, M., Hui, H.-Y. & **Scarola, V. W.** Dynamics of disordered states in the Bose-Hubbard model with confinement. *Phys. Rev. A* **95,** 053624 (2017).

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9. Lin, F., Maier, T. A. & **Scarola, V. W.** Disordered Supersolids in the Extended Bose-Hubbard Model. *Sci. Rep.* **7,** 12752 (2017).

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APPENDIX C- SUPERVISED STUDENTS AND POSTDOCTORAL RESARCHERS

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