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a. REPORT	b. ABSTRACT	c. THIS PAGE			Gregory Fiete
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RPPR Final Report
as of 14-May-2019

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INVESTIGATOR(S):

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Title: Emergent Non-Equilibrium Phenomena in Driven Correlated Materials With Strong Spin-Orbit Coupling

Begin Performance Period: 01-Sep-2014
End Performance Period: 31-May-2018
Report Term: 0-Other

Submitted By: PhD Gregory Fiete
Email: fiete@physics.utexas.edu
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STEM Degrees: 3 **STEM Participants:** 4

Major Goals: The major goal of this project was to theoretically investigate out-of-equilibrium quantum many particle systems that have strong spin-orbit coupling. Particular emphasis was placed on systems with strong correlations. These investigations were carried out with the ultimate aim of finding out-of-equilibrium regimes with interesting properties that might be exploited in applications for the ARO, and DoD more generally. Important progress was made in this direction.

Two examples of out-of-equilibrium regimes with interesting properties are Floquet (periodically driven) systems and pre-thermalized states following a quench to a new Hamiltonian. Both regimes are inherently non-equilibrium and have properties that are quasi-steady state. In a Floquet system, the time averaged (over one period) properties are independent of time, and in the pre-thermalized state there is a time-window of weak time dependence before the system begins to converge more rapidly to a thermal (equilibrium) state. In addition to these two scenarios, we also investigated a quench to a Floquet state: A system initially in equilibrium is suddenly subjected to a periodic drive. This third scenario is a combination of the first two. It turns out (theoretically) that one can obtain an approximate *time- independent* Hamiltonian that describes the dynamics for short-to-intermediate times after the quench to the periodic drive. This observation opens new possibilities for "Hamiltonian engineering" in solid-state systems, and may allow new physical regimes to be opened, possibly in "conventional materials" that are well-known and used in existing applications. To this end, we developed a "flow equation approach" based on renormalization group ideas to obtain such a time-independent effective Hamiltonian.

Accomplishments: Over the course of this project, the PI and his group have been involved with projects in several different areas under the umbrella of non-equilibrium phenomena: (1) Thermoelectric transport in double Weyl semimetals, (2) Disorder effects in correlated topological insulators, (3) Multi-band Floquet systems with quadratic band touching points and flat bands in two dimensions, (3) Topological magnon bands and unconventional superconductivity in pyrochlore iridates, (4) Thermal conductivity of local moment models with strong spin-orbit coupling, (5) Time-dependent dynamical mean-field theory (DMFT) studies of Hubbard models subjected to time-periodic Hamiltonians and (6) The development of a "flow equation approach" to determining the effective time-independent Hamiltonian of a time-periodic system.

The results from topics (1)-(4) were covered in detail in previous reports, so I will focus here on the main results from (5) and (6).

(5) In our time-dependent DMFT studies of Hubbard models we focused on the so-called "mass imbalanced Hubbard model". In this model the hopping (kinetic energy) for spin up and spin down electrons is different. This

behavior is realized in effective models of ferromagnets, and other itinerant magnetic systems, for example. We investigated the behavior of the on-site double occupancy as a function of time and the spin-resolved single electron occupation distribution as a function of time, including the quasi-particle jump. We considered quenches on both the Hubbard interaction and the hopping parameters.

For the mass imbalanced model with a quench on the interactions, we found that when the Coulomb interaction is increased under equilibrium conditions, the quasiparticle weights for spin-up and spin-down (the mass imbalance) electrons approach zero simultaneously, indicating the absence of a spin-selective Mott transition. By contrast, our out-of-equilibrium study of the mass-imbalanced Hubbard model suggests that there exists the spin-selective dynamical phase transition (one spin orientation undergoes a fast thermalization at its critical Coulomb interaction strength while the other spin orientation shows prethermalization behavior). The spin-selective dynamical phase transition is characterized by the relaxation behavior of the spin-resolved kinetic energy and the spin-resolved momentum-dependent occupation. To connect with possible experiments, we calculate the spin-resolved two-time optical conductivity, which confirms the spin-selective thermalization plateau. We find that the critical Coulomb interaction of each spin orientation for the spin-selective thermalization grows as the mass imbalance decreases.

In a separate project, we used nonequilibrium dynamical mean-field theory with iterative perturbation theory as an impurity solver to study the recovery of SU(2) symmetry in real time following a hopping integral parameter quench from a mass-imbalanced to a mass-balanced single-band Hubbard model at half filling. A dynamical order parameter $\gamma(t)$ was defined to characterize the evolution of the system towards SU(2) symmetry. By comparing the momentum-dependent occupation from an equilibrium calculation [with the SU(2) symmetric Hamiltonian after the quench at an effective temperature] with the data from our nonequilibrium calculation, we concluded that the SU(2) symmetry recovered state is a thermalized state. Further evidence from the evolution of the density of states supports this conclusion. We found the order parameter in the weak Coulomb interaction regime undergoes an approximate exponential decay. We numerically investigated the interplay of the relevant parameters (initial temperature, Coulomb interaction strength, initial mass-imbalance ratio) and their combined effect on the thermalization behavior. Finally, we studied evolution of the order parameter as the hopping parameter was changed with either a linear ramp or a pulse. Our results can be useful in strategies to engineer the relaxation behavior of interacting quantum many-particle systems.

In a closely related project to the time-dependent DMFT studies of Hubbard models, we turned our attention to the atomic limit of the on-site part of a multi-orbital Hubbard model. Using exact diagonalization, we studied the spin-orbit coupling and interaction-induced mixing between t2g and eg d-orbital states in a cubic crystalline environment, as commonly occurs in transition metal oxides. We made a direct comparison with the widely used t2g-only or eg-only models, depending on electronic filling. We considered all electron fillings of the d shell and computed the total magnetic moment, the spin, the occupancy of each orbital, and the effective spin-orbit coupling strength (renormalized through interaction effects) in terms of the bare interaction parameters, spin-orbit coupling, and crystal-field splitting, focusing on the parameter ranges relevant to 4d and 5d transition metal oxides. In various limits, we provided perturbative results consistent with our numerical calculations. We found that the t2g−eg mixing can be large, with up to 20% occupation of orbitals that are nominally “empty,” which has experimental implications for the interpretation of the branching ratio in experiments, and can impact the effective local moment Hamiltonian used to study magnetic phases and magnetic excitations in transition metal oxides. Our results can aid the theoretical interpretation of experiments on these materials, which often fall in a regime of intermediate coupling with respect to electron-electron interactions.

(6) In our work on the development of effective time-independent Hamiltonians, we were guided by the high-frequency Floquet expansions which give an effective time-independent Hamiltonian valid in a restricted part of parameter space. To address this limitation, we developed a theoretical method to generate a highly accurate time-independent Hamiltonian governing the finite-time behavior of a time-periodic system. The method exploits infinitesimal unitary transformation steps, from which renormalization group-like flow equations are derived to produce the effective Hamiltonian. Our tractable method has a range of validity reaching into frequency regimes that are usually inaccessible via high frequency ω expansions in the parameter h/ω, where h is the upper limit for the strength of local interactions. We demonstrated our approach on both interacting and non-interacting many-body Hamiltonians where it offers an improvement over the more well-known Magnus expansion and other high frequency expansions. For the interacting models, we compared our approximate results to those found via exact diagonalization. While the approximation generally performs better globally than other high frequency approximations, the improvement is especially pronounced in the regime of lower frequencies and strong external driving. This regime is of special interest because of its proximity to the resonant regime where the effect of a periodic drive is the most dramatic. Our results open a new route towards identifying novel non-equilibrium regimes

and behaviors in driven quantum many-particle systems.

(3) A few other recent projects were focused on on two-dimensional Floquet systems, one in the presence of disorder, and another in the presence of an external magnetic field. These studies helped expand our knowledge of the phenomenology of non-interacting, periodically driven systems. In the disorder project, we found that disorder can induce transitions from topologically non-trivial states to trivial states or vice versa, both examples of Floquet topological Anderson transitions. As a result of the movement of the minimal gap point through the Brillouin zone as a function of laser parameters, the nature of the topological phases and transitions is laser-parameter dependent. In the Floquet Hofstadter butterfly problem, we studi the effect of the laser on the Chern number

Training Opportunities: Two PhD students and one postdoc have been supported on this award in the final reporting period. They have all attended the APS March meeting and given talks, and they have all presented their research at informal seminars in our department. The PI encourages group members to work together, so there have been opportunities for these researchers to guide the progress of younger group members. In addition, group members are encouraged to discuss the results of their research with visitors to our department so that they become familiar explaining their work 1-on-1 to an experienced scientist.

The PI meets regularly 1-on-1 with all group members, and discusses various career opportunities possible with a PhD in theoretical physics. One student has chosen a future career in large scale data analysis. These efforts will help contribute to the overall strength of the US-based technically trained workforce.

Results Dissemination: The following papers have been completed (and copies sent to the ARO program manager of this award) in the final reporting period:

L. Du, Q. Chen, A. D. Barr, A. R. Barr, and G. A. Fiete, ``Floquet Hofstadter Butterfly on the Kagome and Triangular Lattices'', arXiv:1808.02057 (Submitted to PRB)

M. Vogl, P. Laurell, A. D. Barr, and G. A. Fiete, ``A flow equation approach to periodically driven quantum systems'', arXiv:1808.01697 (Submitted to PRX)

H. Nam, C. Zhang, W. Lee, S. Zhu, H.-J. Gao, Q. Niu, G. A. Fiete, and C.-K. Shih, ``Behavior of superconductivity in a Pb/Ag heterostructure with nearly perfect interfacial transparency'', (Submitted to PRL).

L. Du, P. Schnase, A. D. Barr, A. R. Barr, and G. A. Fiete, ``Floquet topological transitions in extended Kane-Mele models with disorder'', Phys. Rev. B {\bf 98}, 054203 (2018).

P. Laurell and G. A. Fiete, ``Magnon thermal Hall effect in kagome antiferromagnets with Dzyaloshinskii-Moriya interactions'', arXiv:1804.09783 (Submitted to PRB)

L. Du and G. A. Fiete, ``Dynamical recovery of SU(2) symmetry in the mass-quenched Hubbard model'', Phys. Rev. B {\bf 97}, 08512 (2018).

G. L. Stamokostas and G. A. Fiete, ``Mixing of t_{2g}-e_g orbitals in 4d and 5d transition metal oxides'', Phys. Rev. B {\bf 97}, 085150 (2018).

Q. Chen, L. Du, and G. A. Fiete, ``Floquet band structure of a semi-Dirac system'', Phys. Rev. B {\bf 97}, 035422 (2018).

L. Du, L. Huang, and G. A. Fiete, ``Orbital-selective thermalization plateau in the mass imbalanced Hubbard model'', Phys. Rev. B {\bf 96}, 165151 (2017).

The works have been discussed and are being discussed in seminars and conference attended by the PI and his group members.

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as of 14-May-2019

Honors and Awards: The PI was awarded a Simons Fellowship from the Simons Foundation. The Fellowship allows the extension of a 6-month sabbatical to a full year. The PI is taking the Fellowship at MIT.

The PI was also elected a Fellow of the American Physical Society (APS) and promoted to Full Professor during this grant period.

Protocol Activity Status:

Technology Transfer: Nothing to Report

PARTICIPANTS:

Participant Type: PD/PI
Participant: Gregory A Fiete
Person Months Worked: 2.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Postdoctoral (scholar, fellow or other postdoctoral position)
Participant: Liang Du
Person Months Worked: 3.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Qi Chen
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Graduate Student (research assistant)
Participant: Georgios Stamokostas
Person Months Worked: 6.00 **Funding Support:**
Project Contribution:
International Collaboration:
International Travel:
National Academy Member: N
Other Collaborators:

Participant Type: Undergraduate Student
Participant: Aaron Barr
Person Months Worked: 2.00 **Funding Support:**
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Other Collaborators:

Participant Type: Undergraduate Student
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ARTICLES:

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Date Submitted: 8/20/18 12:00AM Date Published: 10/30/17 9:00AM
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Article Title: Orbital-selective thermalization plateau in the mass imbalanced Hubbard model
Authors: Liang Du, Li Huang, Gregory A. Fiete
Keywords: Hubbard model, time-dependent DMFT, dynamical phase transition
Abstract: We use time-dependent non-equilibrium dynamical mean-field theory with weak-coupling auxiliary-field continuous time quantum Monte Carlo as an impurity solver to study the thermalization behavior of the mass-imbalanced single-band Hubbard model after a quench of the Coulomb interaction from the non-interacting limit to a finite positive value. By contrast, when the Coulomb interaction in our model is increased under equilibrium conditions, the quasi-particle weight for spin-up and spin-down (the mass imbalance) electrons approach zero simultaneously, indicating the absence of an orbital selective Mott transition. Our out-of-equilibrium study suggests that there exists a time window where an orbital selective dynamical phase transition occurs. The dynamical phase transition is characterized by the relaxation behavior of energy (kinetic and Coulomb interaction) and the spin-resolved momentum-dependent occupation. To make connection with possible experiments, we calculate the spin-res
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Volume: 97 Issue: 3 First Page #: 035422
Date Submitted: 8/20/18 12:00AM Date Published: 1/17/18 5:00AM
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Article Title: Floquet band structure of a semi-Dirac system
Authors: Qi Chen, Liang Du, Gregory A. Fiete
Keywords: Electronic structure, Floquet Systems, Topological materials
Abstract: In this work we use Floquet-Bloch theory to study the influence of circularly and linearly polarized light on two-dimensional band structures with semi-Dirac band touching points, taking the anisotropic nearest neighbor hopping model on the honeycomb lattice as an example. We find that circularly polarized light opens a gap and induces a band inversion to create a finite Chern number in the two-band model. By contrast, linearly polarized light can either open up a gap (polarized in the quadratically dispersing direction) or split the semi-Dirac band touching point into two Dirac points (polarized in the linearly dispersing direction) by an amount that depends on the amplitude of the light. Motivated by recent pump-probe experiments, we investigated the nonequilibrium spectral properties and momentum-dependent spin texture of our model in the Floquet state following a quench in the absence of phonons, and in the presence of phonon dissipation that leads to a steady state independently o
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Article Title: Mixing of eg and t2g orbitals
Authors: Georgios L. Stamokostas, Gregory A. Fiete
Keywords: Hubbard model, multi-obitals, spin-orbit coupling
Abstract: Using exact diagonalization, we study the spin-orbit coupling and interaction-induced mixing between t2g and egd-orbital states in a cubic crystalline environment, as commonly occurs in transition metal oxides. We make a direct comparison with the widely used t2g-only or eg-only models, depending on electronic filling. We consider all electron fillings of the d shell and compute the total magnetic moment, the spin, the occupancy of each orbital, and the effective spin-orbit coupling strength (renormalized through interaction effects) in terms of the bare interaction parameters, spin-orbit coupling, and crystal-field splitting, focusing on the parameter ranges relevant to 4d and 5d transition metal oxides. In various limits, we provide perturbative results consistent with our numerical calculations. We find that the t2g?eg mixing can be large, with up to 20% occupation of orbitals that are nominally “empty,” which has experimental implications for the interpretation of the branching rat
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Article Title: Dynamical recovery of SU(2) symmetry in the mass-quenched Hubbard model
Authors: Liang Du, Gregory A. Fiete
Keywords: Dynamical lattice models, Hubbard Models, phase transition
Abstract: We use nonequilibrium dynamical mean-field theory with iterative perturbation theory as an impurity solver to study the recovery of SU(2) symmetry in real time following a hopping integral parameter quench from a mass-imbalanced to a mass-balanced single-band Hubbard model at half filling. A dynamical order parameter ?(t) is defined to characterize the evolution of the system towards SU(2) symmetry. By comparing the momentum-dependent occupation from an equilibrium calculation [with the SU(2) symmetric Hamiltonian after the quench at an effective temperature] with the data from our nonequilibrium calculation, we conclude that the SU(2) symmetry recovered state is a thermalized state. Further evidence from the evolution of the density of states supports this conclusion. We find the order parameter in the weak Coulomb interaction regime undergoes an approximate exponential decay. We numerically investigate the interplay of the relevant parameters (initial temperature, Coulomb interaction
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Article Title: Floquet topological transitions in extended Kane-Mele models with disorder
Authors: Liang Du, Paul D. Schnase, Aaron D. Barr, Ariel R. Barr, Gregory A. Fiete
Keywords: Disorder, Floquet, topological, phase transition
Abstract: In this work we use Floquet theory to theoretically study the influence of circularly polarized light on disordered two-dimensional models exhibiting topological transitions. We find circularly polarized light can induce a topological transition in extended Kane-Mele models that include additional hopping terms and on-site disorder. The topological transitions are understood from the Floquet-Bloch band structure of the clean system at high-symmetry points in the first Brillouin zone. The light modifies the equilibrium band structure of the clean system in such a way that the smallest gap in the Brillouin zone can be shifted from the M points to the K (K?) points, the ? point, or even other lower-symmetry points. The movement of the minimal gap point through the Brillouin zone as a function of laser parameters is explained in the high-frequency regime through the Magnus expansion. In the disordered model, we compute the Bott index to reveal topological phases and transitions. The disord
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Article Title: Magnon thermal Hall effect in kagome antiferromagnets with Dzyaloshinskii-Moriya interactions
Authors: Pontus Laurell, Gregory A. Fiete
Keywords: Thermal Hall effect, magnons, topological, Chern number
Abstract: We theoretically study magnetic and topological properties of antiferromagnetic kagome spin systems in the presence of both in- and out-of-plane Dzyaloshinskii-Moriya interactions. In materials such as the iron jarosites, the in-plane interactions stabilize a canted noncollinear "umbrella" magnetic configuration with finite scalar spin chirality. We derive expressions for the canting angle, and use the resulting order as a starting point for a spin-wave analysis. We find topological magnon bands, characterized by non-zero Chern numbers. We calculate the magnon thermal Hall conductivity, and propose the iron jarosites as a promising candidate system for observing the magnon thermal Hall effect in a noncollinear spin configuration. We also show that the thermal conductivity can be tuned by varying an applied magnetic field, or the in-plane Dzyaloshinskii-Moriya strength. In contrast with previous studies of topological magnon bands, the effect is found to be large even in the limit of s
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Article Title: A flow equation approach to periodically driven quantum systems
Authors: Michael Vogl, Pontus Laurell, Aaron D. Barr, Gregory A. Fiete
Keywords: Floquet, Effective Hamiltonian
Abstract: We present a theoretical method to generate a highly accurate {\em time-independent} Hamiltonian governing the finite-time behavior of a time-periodic system. The method exploits infinitesimal unitary transformation steps, from which renormalization group-like flow equations are derived to produce the effective Hamiltonian. Our tractable method has a range of validity reaching into frequency regimes that are usually inaccessible via high frequency ? expansions in the parameter h/?, where h is the upper limit for the strength of local interactions. We demonstrate our approach on both interacting and non-interacting many-body Hamiltonians where it offers an improvement over the more well-known Magnus expansion and other high frequency expansions. For the interacting models, we compare our approximate results to those found via exact diagonalization. While the approximation generally performs better globally than other high frequency approximations, the improvement is especially pronounc
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Article Title: Floquet Hofstadter Butterfly on the Kagome and Triangular Lattices
Authors: Liang Du, Qi Chen, Aaron D. Barr, Ariel R. Barr, Gregory A. Fiete
Keywords: Floquet, Hofstadter Butterfly, topological
Abstract: In this work we use Floquet theory to theoretically study the influence of monochromatic circularly and linearly polarized light on the Hofstadter butterfly---induced by a uniform perpendicular magnetic field--for both the kagome and triangular lattices. In the absence of the laser light, the butterfly has fractal structure with inversion symmetry about magnetic flux ?=1/4, and reflection symmetry about ?=1/2. As the system is exposed to an external laser, we find circularly polarized light deforms the butterfly by breaking the mirror symmetry at flux ?=1/2. By contrast, linearly polarized light deforms the original butterfly while preserving the mirror symmetry at flux ? =1/2. We find the inversion symmetry is always preserved for both linear and circular polarized light. For linearly polarized light, the Hofstadter butterfly depends on the polarization direction. Further, we study the effect of the laser on the Chern number of lowest band in the off-resonance regime (laser frequency
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Article Title: Behavior of superconductivity in a Pb/Ag heterostructure with nearly perfect transparency
Authors: Hyoungdo Nam, Chendong Zhang, Woojoo Lee, Siyuan Zhu, Hong-Jun Gao, Qian Niu, Gregory A. Fiete
Keywords: Superconductivity, proximity effect, heterosctructure
Abstract: The superconducting proximity effect, a long-standing topic of great importance in condensed matter physics, has attracted new interest in the context of topological superconductivity and the associated non-Abelian excitations potentially useful in topological quantum computing. A crucial but unresolved issue is which interfacial and material details determine the efficiency of the proximity effect. In this work, we study an epitaxially grown superconductor (SC)/normal metal (NM) heterostructure (Pb/Ag) and show that the electronic transparency is nearly perfect across the interface. We find a spatially constant superconducting gap determined by local tunneling spectroscopy and magneto response measurements, despite the highly mismatched Fermi surfaces between individual Pb and Ag epitaxial layers, and the large differences in the lattice constants and electronic density of states. The uniform superconducting gap is in contrast to the spatially varying pair potential with a discontinui
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Nothing to report in the uploaded pdf (see accomplishments).