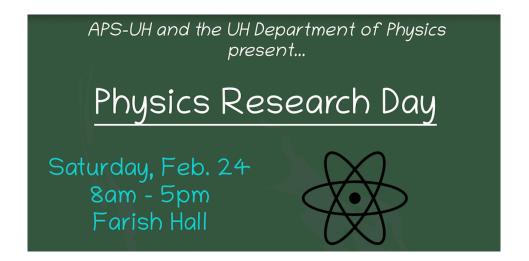
UH Physics Research Day - 2024

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Book of Abstracts

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High Energy and Quantum Field Theory / 2

Critical point fluctuations in heavy-ion collisions within molecular dynamics

Authors: Volodymyr Kuznietsov¹; Volodymyr Vovchenko¹

Co-authors: Horst Stoecker²; Mark Gorenstein; Oleh Savchuk³; Roman Poberezhnyuk⁴; Volker Koch

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We analyze particle number fluctuations in the crossover region near the critical endpoint of a first-order phase transition in baryon-rich matter by utilizing microscopic molecular dynamics simulations of the classical non-relativistic Lennard-Jones fluid. We extend out previous studies by incorporating longitudinal collective flow to model the expansion dynamics in heavy-ion collisions.

In heavy-ion experiments it is possible to observe fluctuations in the momentum space only, so we are concentrating our current research around this topic. The presence of a sizable collective flow is found to be essential for observing large fluctuations from the critical point in momentum space acceptances.

Academic year:

1st year

Research Advisor:

Prof. Volodymyr Vovchenko

Statistical Physics and Condensed Matter and Others $/\ 3$

The Distinct Energy Budgets of Mars and Earth

Author: Larry Guan None

Co-authors: Ellen Creecy ¹; Germán Martínez ²; Liming Li ¹; Matthew Kenyon ³; Xun Jiang ¹

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The radiant energy budget is a fundamental geophysical quantity of great scientific interest for planets and moons. However, detailed studies on the temporal variations of the radiant energy budget for planetary bodies other than Earth are relatively limited. Using thermal and visible measurements obtained from the Mars Global Surveyor spacecraft, we provide the first study on the meridional distribution of Mars'radiant energy budget at seasonal timescales. Our results reveal the dramatic extent of asymmetry in the meridional profiles of Mars'radiant energy budget across seasons, which plays a critical role in the development of large-scale circulation and dust storms on the red planet. This comparative study of radiant energy budget between Mars and Earth reveals marked spatiotemporal dissimilarities. For the annual average radiant energy budget: Mars shows an energy deficit in the tropical region and an energy excess in the middle and high latitudes of both hemispheres.

Earth has the opposite configuration (i.e., an energy excess in the tropics and an energy deficit in middle and high latitudes). The differences in the structure of the radiant energy budget between Mars and Earth have important implications on the general atmospheric circulation and climate of both Earth and Mars.

Academic year:

3rd year

Research Advisor:

Liming Li

High Energy and Quantum Field Theory / 4

Luminosity Detector Studies for the ePIC experiment at the EIC.

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A crucial component to the EIC program is the determination of the collider luminosity. It will be measured through photon emission in the Bethe-Heitler process as it was at HERA. The anticipated high luminosity at the EIC presents several new challenges that necessitate improvements to the base ZEUS pair spectrometer design, which utilizes e+e- conversions of the Bremsstrahlung photons. The new design includes a thin converter foil, sweeper and analyzer magnet, a helium/vacuum chamber, tracking layers, and modern EM calorimeters (Pair Spectrometer Colorimeter). I will present characteristic study of Pair Spectrometer which will provide the first estimate of uncertainties in the measurement of luminosity.

Academic year:

3rd year

Research Advisor:

Prof. Rene Bellweid

High Energy and Quantum Field Theory / 5

Machine Learning Approaches for Phase Transition Recognition in Statistical Models

Authors: Ahmed Abuali^{None}; Claudia Ratti^{None}; David Clarke^{None}; Morten Hjorth-Jensen¹; Ricardo Vilalta²

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We apply Machine Learning (ML) and Deep Learning (DL) techniques to the classification of phase transitions in statistical models, with a focus on binary classification. Our goal is to test whether

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a classification is possible based on configurations only, without the need of calculating an order parameter. The study concentrates on the recognition of phase transitions in prominent spin models such as the 2D Ising model, 3D Ising model, and classical 3D Heisenberg model. The proposed methodology involves training ML and DL models on extensive datasets generated from simulations of the aforementioned statistical models. The training process encompasses diverse configurations representing distinct phases to ensure model generalization. We assess the performance of the models by introducing measures designed to emulate the behavior of an order parameter. These measures serve as indicators of phase transitions, allowing for the discrimination between 1st and 2nd order transitions.

Acad	amic	17001
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		,

3rd year

Research Advisor:

Claudia Ratti

Statistical Physics and Condensed Matter and Others / 6

On a Kneading Theory for Gene-Splicing

Authors: Ethan Speakman Speakman Gemunu Gunaratne

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Two well-known facets in protein synthesis in eukaryotic cells are transcription of DNA to pre-RNA in the nucleus and the translation of messenger-RNA (mRNA) to proteins in the cytoplasm. A critical intermediate step is the removal of segments (introns) containing ~97% of the nucleic acid sites in pre-RNA and sequential alignment of the retained segments (exons) to from mRNA through a process referred to as splicing. Alternative forms of splicing enrich the proteome while abnormal splicing can enhance the likelihood of a cell developing cancer or other diseases. Mechanisms for splicing and origins of splicing errors are only partially known.

Our goal is to determine if rules on splicing can be inferred from data analytics on nucleic acid sequences. We represent a nucleic acid site as a point in a plane defined in terms of the anterior and posterior sub-sequences of the site. It is found that point-sets for exons and introns are visually different, and that the differences can be quantified using a family of generalized moments. We design a machine-learning algorithm that can recognize individual exons or introns with 91% accuracy. Point-set distributions and generalized moments are found to differ between organisms.

Academic year:

4th year

Research Advisor:

Gemunu Gunaratne

Material Science / 10

Study of the Thermoelectric properties of n-type Mg3Sb2 via doping Zr and incorporating MXene

Author: Suraj Pradhan^{None}

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In recent times, there has been a growing interest in thermoelectric Zintl compounds due to their excellent thermoelectric performance across various families. Among these, Mg3Sb2-based Zintl compounds have garnered attention as potential thermoelectric materials. However, their effectiveness is hindered by weak electrical transport properties stemming from their p-type nature. The poor electrical transport characteristics of p-type Mg3Sb2 can be attributed to its high thermal conductivity, low hole concentration, and relatively large band gap of 1.23 eV, primarily resulting from the presence of Mg vacancies. Nevertheless, an excess of Mg can reduce these vacancies, transforming the material into an n-type compound with superior electrical transport properties, thereby making it a more promising candidate for thermoelectric applications. Consequently, n-type Mg3Sb2-based materials have emerged as viable options for temperatures ranging from 300 K to 773 K, owing to their high band degeneracy, low lattice thermal conductivity, low toxicity, and abundance. Among these materials, Te-doped Mg3+xSb1.5Bi0.5 stands out as particularly promising, as the excess Mg combined with moderate Te doping enables the regulation of carrier type and concentration. Notably, Tamaki et al. demonstrated that a sample with a composition of Mg3.2Sb1.5Bi0.49Te0.01 achieved a remarkable figure of merit of zT 1.5 at 716 K. Our objective here is to further enhance the thermoelectric properties of n-type Mg3.2Sb1.5Bi0.49Te0.01 through doping and forming a composite.

Academic year:

3rd year

Research Advisor:

Dr. Zhifeng Ren

Material Science / 12

Ultrafast Electron Diffraction Studies in the Two-Dimensional Magnet CrSBr

Author: Jayajeewana Ranhili Pelige¹

Co-authors: Alberto Ruiz ²; Byron Freelon ¹; John Cenker ³; Jose Baldovi ²; Junjie Li ⁴; Ka Shen ⁵; Mark Palmer ⁴; Mikhail Fedurin ⁴; Sumit Khadka ¹; Xiaodong Xu ³

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Ultrafast Electron Diffraction Studies in the Two-Dimensional Magnet CrSBr

CrSBr is an air-stable, novel two-dimensional (2D) magnetic van der Waals (vdW) single crystal that received intense study as a future spintronics material. The material shows some interesting properties such as a large optical band gap (~ 1.5 eV), strong spin-phonon coupling (SPC) effect, quasi 1-D electronic structure, strain-induced magnetic phase transitions, and enhanced structural deformability. In our work, mega-electron volt (MeV) ultrafast electron diffraction (UED) was employed to investigate the ultrafast structural dynamic response of this material. We observed femtosecond pump pulses excited small anisotropic lattice deformations that are to be mediated by coherent acoustic phonons (CAPs). The phonons were interpreted as longitudinal breathing modes. The ultrafast oscillatory behavior of Bragg peak intensities was simulated by incorporating an oscillating deviation parameter ansatz into dynamical scattering intensity expressions. This allowed for excellent modeling of the ultrafast structural dynamics of the photo-excited 2D crystalline membranes. The phonon frequencies were extracted by analyzing these oscillations in Bragg peak intensities and

they were in nearly 23 GHz range. These results suggest a promising path for tuning the ultrafast photo-induced properties of CrSBr with sample geometry and dimension.

Academic year:

5th year and/or beyond

Research Advisor:

Dr. Byron Freelon

Poster Session / 13

Effects of Protein Crowders and Charge on the Folding of Superoxide Dismutase1 (SOD1) Variants: A Computational Study

Author: Atrayee Sarkar¹

Co-authors: Andrei G. Gasic 2; Margaret S. Cheung 3; Greg Morrisson 4

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Mutations in the Superoxide Dismutase 1 (SOD1) protein may cause misfolding and aggregation leading to the neurodegenerative disease ALS. Despite numerous studies a clear understanding of the impact of electrostatics and crowding on the folding and aggregation of SOD1 remains lacking. In this work, we use a structure-based model and molecular dynamics simulation to study the effects of electrostatics on SOD1 folding in a crowded environment. We show that electrostatics affect the unfolded protein configurations more significantly than the folded ones. Using a new order parameter, we suggest the presence of an intermediate state and show that electrostatics play an important role in the folding pathway of SOD1.

Academic year:

5th year and/or beyond

Research Advisor:

Dr. Greg Morrison

Poster Session / 14

Finite density QCD equation of state: critical point and lattice-based T^\prime -expansion

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We present a novel construction of the QCD equation of state (EoS) at finite baryon density. Our work combines a recently proposed resummation scheme for lattice QCD results with the universal critical behavior at the QCD critical point. This allows us to obtain a family of equations of state in

the range $0 \le \mu_B \le 700$ MeV and 25 MeV $\le T \le 800$ MeV, which match lattice QCD results near $\mu_B = 0$ while featuring a critical point in the 3D Ising model universality class.

The position of the critical point can be chosen within the range accessible to beam-energy scan heavy-ion collision experiments. The strength of the singularity and the shape of the critical region are parameterized using a standard parameter set.

We impose stability and causality constraints and discuss the available ranges of critical point parameter choices, finding that they extend beyond earlier parametric QCD EoS proposals. We present thermodynamic observables, including baryon density, pressure, entropy density, energy density, baryon susceptibility and speed of sound,

that cover a wide range in the QCD phase diagram relevant for experimental exploration.

Academic year:

4th year

Research Advisor:

Prof. Claudia Ratti

High Energy and Quantum Field Theory / 15

Improving Calibration Methods for NOVA Experiment

Author: Dat Tran¹

Co-author: Lisa Koerner 2

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The NuMI Off-Axis nu_e Appearance (NOvA) is an experiment designed to study neutrino oscillations. It utilizes two detectors, one located in Batavia, Illinois (the near detector), and the other one located in Ash River, Minnesota (the far detector). NOvA's neutrino oscillation analyses require precise correlation of events in the detector with the narrow 10 μ s NuMI neutrino beam pulses. The technique to calibrate the timing system uses the cosmic-ray muon flux at the detector's surface location to establish a precise network of timing offsets between the detector components spread over the 64 m spatial extent of the detector. Cosmic-rays are also used to measure the light yield and attenuation

length within the detector cells and to establish the absolute energy

scale of the detector. This talk will cover recent upgrades to the methods of calibration used in the NOVA experiment.

Academic year:

3rd year

Research Advisor:

Lisa Koerner

Statistical Physics and Condensed Matter and Others / 16

Finding Community Structure in Networks with RenEEL and its Extension to Bipartite Networks

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Arguably the most fundamental problem in Network Science is finding structure within a complex network. One approach is to partition the nodes into communities that are more densely connected than one expects in a random network. "The" community structure corresponds to the partition that maximizes a measure that quantifies this idea. Finding the maximizing partition, however, is a computationally difficult NP-complete problem. We explore the use of a recently introduced algorithmic scheme [Guo, Singh, and Bassler, Sci. Rep. 9, 14234 (2019)] to find the structure of a set of benchmark networks. The scheme, known as Reduced Network Extremal Ensemble Learning (RenEEL), creates an ensemble of k partitions and updates the ensemble by replacing its worst member with the best of k' partitions found by analyzing a simplified network. The updating continues until consensus is achieved within the ensemble. Varying the values of k and k', we find that the results obey different classes of extreme value statistics and that increasing k is generally much more effective than increasing k' for finding the best partition. Building upon this exploration, we propose to extend the methodology addressed in [Guo, Singh, and Bassler, J. Phys. Complex. 4 (2023) 025001] to bipartite networks. Introducing a novel metric, bipartite generalized modularity density Q_{bg} . This function has a tunable parameter that sets the scale for the typical community found. By varying this parameter hierarchical structure can be found in bipartite networks.

Academic year:

4th year

Research Advisor:

Dr. Gemunu Gunaratne, Dr. Kevin E Bassler

High Energy and Quantum Field Theory / 17

Entanglement Entropy in p-p Collisions at LHC Energies

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In an effort to better understand the thermal-like behavior and particle yields seen in p-p collisions we recast the problem employing the principles of quantum states and their entanglement in the produced system. We seek to show that this entanglement in the initial state has a measurable effect on the evolution of the system and is the driving mechanism behind the thermal-like behavior and particle yields observed. Recent studies have demonstrated that entanglement in the initial state could endure the evolution of a strongly coupled system. Consequently, we attempt to show equivalence in a calculation of the initial state entropy (calculated using PDF's) and the final state entropy (calculated using multiplicity distributions). Multiplicity distributions used in this study are that of primary charged particles, measured using the ALICE detector at the LHC.

Academic year:

5th year and/or beyond

Research Advisor:

Rene Bellwied

¹ University of Houston

¹ University of Houston (US)

Poster Session / 18

Introduction to Single-Mask X-ray Phase Contrast Imaging

Author: Jingcheng Yuan^{None}

Co-author: Mini Das ¹

¹ University of Houston

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Traditional X-ray imaging methods often struggle to capture detailed structures within soft tissues due to their limited contrast capabilities. In response, this study introduces Single-Mask X-ray Phase Contrast Imaging (PCI), a pioneering technique aimed at enhancing the visualization of subtle tissue differences. Our focus lies in the single-mask approach, which utilizes a periodic X-ray absorption mask to introduce contrast-enhancing effects. Central to our methodology is a novel model that elucidates the intricate interplay between X-ray attenuation, Laplacian phase, and differential phase contributions to detector pixel intensities. We present a streamlined retrieval method capable of extracting both attenuation-based and differential phase contrast information in a single acquisition, significantly expanding imaging capabilities. This breakthrough holds immense potential for revolutionizing medical diagnostics and beyond, paving the way for new frontiers in non-invasive imaging technology.

Academic year:

5th year and/or beyond

Research Advisor:

Mini Das

Poster Session / 19

Evolution with Information-Based Fitness

Author: Yi-Kai Mo^{None}

Corresponding Author: ymo6@uh.edu

The mechanisms through which evolution shapes biological organisms remain a mystery. It has been hypothesized that organisms evolve to increase their information. We consider the evolution of a population of Boolean networks, which we take as models of gene regulatory networks, through an evolutionary game framework utilizing mutation and fitness. Fitness is a function of the mutual information (MI) in gene expression over the attractor of the network's dynamics. By studying the symmetry of the Boolean functions in the networks, we show that there exists a phase transition in the evolved state as the rate of mutation changes.

Academic year:

3rd year

Research Advisor:

Dr. Kevin E Bassler

Material Science / 20

Replication and study of anomalies in LK-99, the alleged ambientpressure, room-temperature superconductor

Authors: Thacien Habamahoro¹; Trevor Bontke²; Meiraba Chirom³; Zheng Wu²; Jiming Bao⁴; Liangzi Deng¹; Ching Wu Chu¹

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Corresponding Author: thabamahoro@uh.edu

The unique simultaneous appearance of zero resistivity and magnetic field expulsion enable superconductors to have tremendous potential for various applications, such as efficient electric power transmission, much smaller or more powerful magnets, magnetic levitation, high-speed computing, etc. The superconducting critical transition temperature (Tc) has continuously been enhanced owing to the century-old effort at superconductivity. It appears that all record high Tcs since 1994 have been achieved in compounds under very high pressure. The ultimate goal in the superconductivity field is to find a way to retain a coherent quantum state under ambient conditions, i.e., room temperature of ~ 300 K and atmospheric pressure. We have studied LK-99 [Pb10-x Cux(PO4)6O], alleged by Lee et al. to exhibit superconductivity at room temperature and ambient pressure, and have reproduced all the anomalies except for half-levitation they reported as evidence for the claim of LK-99 being an ambient-pressure, room-temperature superconductor. We found that these anomalies are associated with the structural transition of the Cu2S impurity in their sample and not with superconductivity.

Academic year:

3rd year

Research Advisor:

Prof. Ching Wu Chu

High Energy and Quantum Field Theory / 21

Dual-Phase TPC Separation Grid Development and Production in Darkside-20k Prototypes

Author: Daniel Huff¹

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A plurality of collaborations around the world today employ time projection chambers (TPCs) in highly sensitive detectors to search for evidence of rare particles. The dual-phase TPC detector concept relies on two unique (but related) event signals, S1 and S2, to increase a detector's robustness against background influences. The Darkside-20k experiment applies this idea to the pursuit of dark matter detection. In its detectors, Darkside-20k utilizes an S1 signal from recoil-induced photon emissions in liquid Argon, and an S2 signal from orchestrated collisions between ionization electrons and the "second phase" gas pocket of the TPC. A uniform electric drift field is applied to the lower liquid volume to direct ejected electrons towards a separation grid; there a stronger second field accelerates them into a region of gas particles. The separation grid is carefully designed and constructed to ensure field uniformity through physical symmetry and resistance to destructive forces from the detector. A wound-pin technique is used to produce suitable grid wire units from stainless steel which can maintain this function.

Academic year:

3rd year

Research Advisor:

Andrew Renshaw

Material Science / 22

PTFE reinforced electrolyte membrane for high performance and durability in proton exchange membrane fuel cell (PEMFC)

Author: Subash Bhandari^{None}

Co-authors: Anima Bose; Dinh Cong Tinh Vo Corresponding Author: scbhandari@uh.edu

Hydrogen fuel cells have proven to be the best alternative to fossil fuels for ecofriendly and high performing clean power generation. Among the various types of fuel cells, proton exchange membrane fuel cell (PEMFC) has demonstrated a wider range of applications mainly because of low operating temperature (50 oC -80 oC), high efficiency, and higher power range (1KW -100 KW). In PEMFC, the electrolyte membrane plays a vital role for its performance and durability. A type of perfluoro sulfuric acid (PFSA) based membrane, Nafion® by Dupont, is the state-of-the-art (SOA) electrolyte membrane for PEMFC over 50 years, however, it offers relatively lower durability due to high swelling at hydrated stage, low mechanical strength, gas permeability, and unstable proton conductivity under harsh conditions. Recently, an advanced electrolyte membrane with high dimensional stability has been developed in our laboratory by incorporating PFSA ionomer solution into the porous poly(tetrafluoroethylene) (PTFE) substrate. The idea was to develop a robust electrolyte membrane with low PFSA content and resolve some drawbacks of Nafion® membrane. In the membrane designing process, the issue of incompatibility between hydrophobic PTFE and hydrophilic PFSA polymer interface was addressed by surface modification of PTFE substrate with semi-hydrophilic material. The developed composite membrane exhibits significantly improved properties compared to the Nafion® membrane. For instance, the swelling ratio reduced by 60% and the proton conductivity increased by higher than 20%. The prepared membrane was tested in single cell PEMFC setup where it demonstrated excellent performance with peak power density of 1670 mW cm 2, which was more than 50% higher compared to Nafion® membrane. The composite membrane also performed very well in low hydrated state and showed longer durability demonstrating the superiority over SOA Nafion® membrane.

Academic year:

4th year

Research Advisor:

Anima Bose

Material Science / 23

Band Topology of LK-99

Author: Bishnu Karki^{None}

Co-authors: Kai Chen 1; Pavan Hosur 1

¹ University of Houston

Corresponding Author: bkarki2@uh.edu

Recent reports of room temperature ambient pressure superconductivity in LK-99 sparked tremendous excitement. While the materials is no longer believed to be superconducting, interest in its electronic and topological properties of the material still stands. Here, we utilize first-principle density functional theory and augment a recently proposed model tight-binding Hamiltonian to study the band topology including the impact of spin-orbit coupling. In the absence of spin-orbit coupling, we observed the presence of two isolated bands situated near the Fermi level. However, upon the introduction of spin-orbit coupling, these two bands split into four bands and generate multiple Weyl points with Chern number ±2. We also observe accidental crossings along high symmetry lines which, at the level of our minimal Hamiltonian, extend as nodal surfaces away from these lines.

Academic year:

3rd year

Research Advisor:

Dr. Pavan Hosur

Statistical Physics and Condensed Matter and Others / 24

Superconductor vortex spectrum in type 2 Weyl semi metal

Author: Swadeepan Nanda^{None} **Co-author:** Pavan Hosur ¹

Corresponding Author: snanda3@uh.edu

Recent discoveries of pressure-influenced superconducting critical temperature(Tc) in semi-metallic transition metal dichalcogenides(WTe2, MoTe2) have intrigued deep research on TMDs. Both the semi-metallic TMDs have been found to host the Weyl semi-metal phase with tilted Weyl nodes. Using a semiclassical picture to bypass the hurdle of bulk-surface inseparability, we derive the superconductor vortex spectrum in non-magnetic Weyl semimetals with tilted Weyl nodes and show that it stems from the Berry phase of orbits in the continuum limit. We have found that upon tilting the vortex, the existence of zero modes depends on the vortex tilt: if the vortex tilts beyond that of the Weyl nodes, there is no Majorana zero mode.

Academic year:

4th year

Research Advisor:

Pavan Hosur

Statistical Physics and Condensed Matter and Others / 25

Decomposition of Anomalous Diffusion in Variable speed generalized Lévy Walks

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¹ University of Houston

Co-author: Kevin Bassler 1

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Diffusive behavior is normally governed by the Central Limit Theorem (CLT), which states that the displacement in the limit of large time has a Gaussian distribution with a width that increases as square root of time. However, diffusive behavior that differs from the CLT is found in a wide array of experimental systems. The root causes of anomalous diffusive behavior can be identified by decomposing the behavior into three fundamental constitutive effects, each of which are associated with the violation of an assumption of the CLT and are known as the Joseph, Noah, and Moses effects. The dynamics of systems with anomalous diffusive behavior can be modeled with Variable speed generalized Lévy Walks (VGLWs) that have steps of random duration chosen from a power law probability distribution and a velocity in each step of magnitude deterministically non-linearly coupled to the intended flight duration and actual time in motion. Here, we decomposed the anomalous diffusion caused by VGLWs, finding that the anomalous diffusive behavior is generally a complex combination of the three constitutive effects. We also found that we can access non-scaling regime of generalized Lévy Walks in VGLWs and show that the Latent exponent L that characterizes the Noah effect has no upper bound.

Academic year:

4th year

Research Advisor:

Kevin Bassler

High Energy and Quantum Field Theory / 26

The fixed-target experiment in STAR @ RHIC

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The RHIC Beam Energy Scan (BES-I) program, which covers center-of-mass energies 7.7 GeV to 39 GeV, was proposed to look for the turn-off of signatures of the quark gluon plasma, search for a possible QCD critical point, and study the nature of the phase transition between hadronic and partonic matter. RHIC BES-I has shown that the partonic interactions are dominant at center-of-mass energies above 20 GeV.

Several observables, including v1 of protons and Lambdas, v2 of all identified hadrons, and netproton higher moments, show interesting behavior below 20 GeV and could suggest a transition to a hadron interaction dominated regime. Data from energies lower than 7 GeV

could help determine whether these behaviors are indicative of phase transitions or criticality. The goal of the STAR Fixed-Target Program is to extend the collision energy range in BES

II to lower energies than what is feasible at RHIC with colliding beams. The implications for the fixed-target program after the completion of the inner TPC (iTPC) and endcap TOF (eTOF) detector upgrades will also be discussed.

Academic year:

3rd year

Research Advisor:

Rene Bellwied

¹ University of Houston

Material Science / 27

Spectroscopic Study of the Electronic Structure in Two-dimensional Chromium trihalides

Authors: Amol Singh¹; Byron Freelon²; Chamini Pathiraja²; Christian Schulz³; Deniz Wong³; Di-Jing Huang⁴; Hsiao-Yu Huang¹; Jayajeewana Ranhili Pelige²; Yi-De Chuang⁵; Yu-Cheng Shao¹

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The recent discovery of ferromagnetism in 2D van der Waals Chromium trihalides CrX_3 (X = Cl , Br and I) down to the monolayer has gain research attraction because of their interesting electronic and magnetic properties. The magnetic properties of CrX_3 can be manipulated by applying perturbations such as external magnetic field, strain, pressure. This makes CrX_3 prime candidates for spintronics and magneto-resistive memory applications. Understanding the magnetism also appears to be linked to determining the electronic levels of Cr bands near the Fermi energy. These circumstances suggest that obtaining precisely determined energy scales is a prerequisite for constructing theoretical models that explain the magnetic ground states of CrX_3 . High-resolution, soft x-ray can provide improved spectral features beyond the numerous techniques previously applied to these well studied metal halide systems. We have measured Cr L-edge soft x-ray absorption spectroscopy (XAS) and resonant inelastic x-ray scattering (RIXS) spectroscopy for all CrX_3 in order to understand their electronic structure. Through a systematic study, with the use of atomic multiplet simulations, we show that our approach has yielded a set of more reliably determined energy scale parameters. Ultimately, our goal is to achieve a detailed understanding of the electronic structure of CrX_3 and determine how it is related to magnetic order and excitations in these fascinating systems.

Academic year:

5th year and/or beyond

Research Advisor:

Byron Freelon

Material Science / 28

Synthesis of Ce-doped NiFe-LDH electrocatalysts for oxygen evolution reaction through a single-step hydrothermal method

Authors: Byaruhanga Paul¹; Yu Wang²; Vidhi Vidhi¹; Shuo Chen¹

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Pursuing hydrogen fuel via water electrolysis has attracted much attention to overcome the diminishing reserves of fossil fuels and their environmental repercussions. The efficiency of water electrolysis largely hinges on overcoming the inherently sluggish kinetics of oxygen evolution reaction (OER). Innovating highly active, durable, cost-effective OER electrocatalysts is essential, especially in alkaline environments. NiFe-layered double hydroxides (LDH) hold promise as one of the most active electrocatalysts for the OER in alkaline environments. Nonetheless, its advancement demands

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improved activity and stability under harsh alkaline conditions. Unlike previous studies, we synthesized cerium-doped NiFe-LDH nanosheets through a single-step hydrothermal method. Introducing cerium in place of iron atoms boosts the catalytic efficiency and enriches the materials with more active sites. Our optimized Ce-doped NiFe-LDH/NF electrocatalyst demonstrated remarkable OER activity, requiring overpotentials of just 247 mV and 304 mV to achieve current densities of 100 and 1000 mA cm-2, respectively, with a low Tafel slope of 34.5 mV dec-1 in 1 M KOH. Notably, the electrocatalyst exhibited exceptional stability, maintaining robust performance in up to 6 M KOH solutions at room temperature and 65 oC, respectively, for about 300 h at elevated current densities of 500 mA cm-2, outperforming all the Ce-doped catalysts reported before in both performance and stability tested under identical conditions. These results underline the potential of Ce-doped NiFe-LDH as a cost-effective and highly efficient catalyst for sustainable hydrogen production, highlighting the importance of the one-step synthesis approach in advancing electrocatalytic materials.

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ricuu	CILLE	y cur.

3rd year

Research Advisor:

Shuo Chen

Poster Session / 29

Investigating the Magnetic Ordering of Strained CrSBr by Neutron Diffraction

Author: Uchenna Ubeh^{None}

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Since the discovery of graphene, two-dimensional (2D) materials have sparked great interest among condensed matter physicists. These materials exhibit new physical properties, and their magnetic versions promise numerous applications for spintronics, optoelectronic devices, and quantum computing hardware. 2D magnets are attractive on their own, but the van der Waals (VdW) form has exhibited new and exotic effects. One example is Chromium Sulphur Bromide (CrSBr), which has been shown to be multi-functional and air-stable among magnetic 2D magnets.

The recent discovery of 2D VdW magnets provides a new platform for manipulating magnetic properties with versatile methods to control, including electric and nanomechanical means. Strain ϵ engineering is a practical approach to tuning fundamental properties of 2D materials. Examples include the strain control of nematic, superconducting, and topological phases by modifying a given crystal's lattice constant and symmetry. Strain can also influence the magnon's VdW magnets. Strain has been shown to change the lattice structure and affect the exchange interaction between magnetic ions, leading to changes in the magnon spectrum and the magnon density of states. Theoretical studies have suggested that strain can modify magnetic ordering and magnetic anisotropy. We have designed a custom strain mount that will allow us to strain our CrSBr, thereby tuning its magnetic ordering mechanically. Our work will create new opportunities to harness the power of a strain control system to study the structural properties and magnetic order of CrSBr using neutron diffraction.

Academic year:

4th year

Research Advisor:

Dr. Byron Freelon

High Energy and Quantum Field Theory / 30

Extrapolation of baryon density contours to search for the QCD critical point.

Author: Hitansh Shah^{None}

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Lattice QCD calculations show that there is an analytic crossover from hadron resonance matter to a deconfined quark gluon plasma at vanishing baryon chemical potential. Many models predict that this analytic crossover changes to a line of first order phase transition at finite baryon chemical potential with a critical point. Due to the Fermi sign problem, we cannot have the lattice calculations at finite chemical potential, which is why there are several models that try to find the critical point. Here, we are trying to have an extrapolation in positive chemical potential by looking at contours of baryon density, which near the phase transition should overlap on each other and give us the spinodal region. Firstly, we will be working on Van der Waals model in both canonical and grand canonical ensemble and look how this extrapolation works and give us the phase transition and then project on to the QCD phase diagram.

Academic year:

3rd year

Research Advisor:

Claudia Ratti

Statistical Physics and Condensed Matter and Others / 31

Measurement Induced Logical Qutrits in Kitaev Honeycomb Circuit

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Inspired by Kitaev's Honeycomb Model, we take a qutrit honeycomb circuit and perform repeated measurements to find that when the probability of pz» px, py, it encodes a logical qutrit.

Academic year:

5th year and/or beyond

Research Advisor:

Dr. Pavan Hosur

High Energy and Quantum Field Theory / 32

ALICE Experiment In LHC Run 3

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At the Large Hadron Collider (LHC), at CERN, we are able to create the hottest and the densest conditions which are similar to those at the beginning of the Universe. During the past ten years, we observed the existence of Quark Gluon Plasma (QGP) which is formed at the early stages of heavy ion collisions. The measurements we obtained led to significant progress for understanding its properties through Pb-Pb or Xe-Xe collisions, but also from even smaller systems such as p-Pb. During the Long Shutdown 2, ALICE experiment undergone major upgrades for both hardware and software components. On July 5^{th} 2022, LHC entered in the era of Run 3 establishing a milestone for ALICE which will collect data at an interaction rate 50 times larger than before. The two main goals are to record data much faster comparing with Run 1 & 2, and to enhance the track reconstruction efficiency and precision for the detection of short-lived particles containing heavy-flavour quarks. ALICE detector has close to 13 billion electronic sensor elements with a continuous read out, creating a data stream of more than 3.4 terabytes per second. The new computing scheme for Run 3 replaces the traditionally separate online and offline frameworks by a unified one, which is called O^2 . Around 500 billion minimun bias events of p-p collisions were collected during 2022, and about 12 billion reconstructed events of five weeks Pb-Pb in 2023.

Academic year:

4th year

Research Advisor:

Anthony R. Timmins

Poster Session / 33

Promotional Effect of Fe2+ in the electrocatalytic activity of FeMoO4 nanorod array for Oxygen Evolution Reaction under Alkaline Conditions

Author: Vidhi Vidhi¹
Co-author: Shuo Chen ²

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Electrochemical water splitting emerges as a pivotal strategy for sustainable hydrogen energy production. Alkaline water electrolysis offers a facile pathway to yield pure hydrogen. However, due to its intrinsically sluggish kinetics, the anodic oxygen evolution reaction (OER) poses a formidable challenge. Overcoming this hurdle demands efficient water oxidation electrocatalysts to mitigate overpotential and enhance overall efficiency. While state-of-the-art catalysts such as RuO2 and IrO2 excel in OER catalysis, their limited availability and high cost impede broader implementation.

Transition metal compounds, encompassing elements such as Cu, Fe, Ni, Co, W, and Mo, have emerged as intriguing candidates for catalyzing the oxygen evolution reaction (OER). Notably, materials rooted in Mo and Fe, exemplified by MoS2, Mo2C, MoB2, MoP, MoOx, FeC, and FeOx, have undergone thorough examination owing to their tunable electronic configurations and robust structural integrity, rendering them promising for applications in water electrolysis. Utilizing a hydrothermal synthesis method, FeMoO4 supported over Nickel Foam (NF) substrate was synthesized. Characterization techniques including X-ray diffraction and scanning electron microscopy revealed crystalline nanorods of the FeMoO4 moieties which provide a large surface area for the OER. Cyclic voltammetry of samples incorporating ferrous salts as the Fe2+ precursors enhanced the OER performance compared to its conventional counterparts having Fe3+. In an alkaline oxidative environment of OER, Fe2+ having a partially filled 3d6 electronic configuration makes it less stable and hence more

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reactive than Fe3+. This work presents an overpotential of 229 and 251 mV at 10 and 50 mA/cm2 respectively which is much lower than recently reported a noble metal oxide electrocatalyst like IrO2/NF (290 mV at 10 mA/cm2) and RuO2/NF (263 mV at 50 mA/cm2). These findings underscore the potential of FeMoO4 as a cost-effective and promising candidate for advancing the field of water oxidation in electrochemical water splitting.

Academic year:

2nd year

Research Advisor:

Dr. Shuo Chen

Poster Session / 34

Atmospheric neutrino zenith angle and non-standard interaction study

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Introduction to neutrino oscillation, atmospheric neutrino, NOvA experiment and non-standard neutrino interaction on atmospheric neutrinos.

Academic year:

5th year and/or beyond

Research Advisor:

Lisa Koerner

Poster Session / 35

Development and characterization of advanced nanomaterials for chemical sensing.

Authors: Lilly Schaffer¹; Maggie Paulose¹; Waligo David^{None}

Co-author: Oomman K. Varghese

¹ Department of Physics

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In recent years, gas sensors have been increasingly used in daily life to enhance the ability of human beings to perceive the surroundings. Gas sensors are commonly used for process automation, dangerous gas leak detection, environmental pollution monitoring, and breath analysis to identify drunk driving. Metal oxide gas sensors utilize changes in the electrical conductivity of semiconducting oxides (e.g. TiO2, SnO2) with respect to target gas concentrations for operation. Low cost, fast response, simple design, and potential to detect gases in low concentrations are their highly desirable attributes. Recently, there have been efforts to use these sensors for medical diagnosis via detection

of volatile organic compounds (VOCs) in breath. Nevertheless, exhaled air contains hundreds of VOCs in low concentrations (parts per million to trillion level) and detecting them with high specificity from this complex environment is challenging. We could address this problem by developing unique nanostructured materials and utilizing machine-learning techniques. In this presentation, we discuss the performance of a sensor array based on advanced nanomaterials in detecting cancer related VOCs.

Academic year:

4th year

Research Advisor:

Oomman K. Varghese

Statistical Physics and Condensed Matter and Others / 36

Physics-Inspired Modeling and Validation Approaches for Pharmaceutical Security

Author: Timothy Burt¹

Co-authors: Abhijit Bera ¹; Andres Covarrubias ¹; Ioannis Kakadiaris ¹; Nikos Passas ²

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We discuss our plans to incorporate strategies from physics into AI-SNIPS (AI-Support for Network Intelligence-Based Pharmaceutical Security), a cloud-based platform designed for the domain of Illicit, Substandard, and Falsified Medical Products (ISFMP) that enables stakeholder decision-making, secure data sharing, and interdisciplinary research. The project is separated into software engineering (frontend/backend web development) and research modules. The first part of the talk will summarize our research findings using two static datasets collected from web scraping URLs provided by our stakeholders. The remainder of the talk will discuss two modules currently in the planning phase: dynamics and disruptions (validation of targeting strategies and node/edge failures). A key finding is that a natural period of about two weeks in the availability of ISFMP items emerges regardless of lead type or initial scraping date. It is necessary to capture and model time-series data and changes in ISFMP availability to evaluate various disruption strategies in collaboration with our stakeholders. We emphasize that this project does not involve any illicit drugs or drug paraphernalia, only FDA-approved products sold by pharmaceutical companies, nor does it involve disruptions of ISFMP activity, as that is the job of law enforcement. By validating the best strategies to address the root problem of ISFMP and pharmaceutical counterfeiting, hundreds of thousands of lives can be saved each year worldwide due to the proliferation and sale of these items in our society.

Academic year:

5th year and/or beyond

Research Advisor:

Ioannis Kakadiaris

Poster Session / 37

¹ University of Houston

² Northeastern University

Investigating the efficiency of mixing in centrifuge tube based on novel ultrasonic generator.

Author: Paththini Kuttige nonis1

Co-authors: Di Chen ²; Elizabet Rosas ; Jiming Bao ³; Jon MIcheal ; Tian Tong ¹; Wei- Kan Chu ⁴

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This paper illustrates a liquid mixing device that generates ultrasonic waves through shining pulse laser of a Gold implanted fiber optic cable and uses the laser streaming to accomplish the mixing liquids with different viscosities in centrifuge tube. Pure gold nanoparticles were implanted beneath the surface of the glass fiber optics cable. The pulse laser (527nm wavelength) was used to generate the liquid jet out of the tips of Au implanted glass fiber optics cable. The mixing experiment was done using Au-implanted optics tip suspension in centrifuge tubes of two different viscous liquids. Here we have investigated the behavior of laser streaming, after and before heat treatment of the Au-implanted quartz plate, and how the speed of the laser streaming varies with the viscosity of the solution.

Academic year:

4th year

Research Advisor:

Wei-Kan Chu

Statistical Physics and Condensed Matter and Others / 38

Generalized Free Cumulants for Quantum Chaotic Systems

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The eigenstate thermalization hypothesis (ETH), the leading conjecture for the emergence of statistical mechanics in quantum systems, is formulated in terms of matrix elements of observables. However, much stronger statements about chaotic systems are available from the structure of their eigenstates. The ETH has recently been reinterpreted in terms of the mathematical subject of free probability theory. I discuss this connection and argue that its extension to chaotic eigenstates yields a powerful diagrammatic framework whose connected components I refer to as generalized free cumulants. Using these diagrams, I discuss how time-dependent quantities such as reduced density matrices and entanglement entropy reach thermal equilibrium and provide insight into the Page curve for entanglement entropy.

Academic year:

3rd year

Research Advisor:

Pavan Hosur

Poster Session / 39

Improving the Numu-CC1Pi Cross Section on Water at T2K

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The T2K experiment is designed to study neutrino oscillations and the associated oscillation parameters. It utilizes a set of two detectors, the near detector is located near the beam target in Tokai, Japan and the far detector is located in Kamioka, Japan. Since the far detector (SK) uses Water-Cherenkov radiation to detect outgoing particles from a neutrino interaction, constraining the cross sections of different neutrino interaction types on water is required. This talk will highlight some of the updates made to the CC1Pi Cross Section measurement.

Academic year:

5th year and/or beyond

Research Advisor:

Dr. Daniel Cherdack

Statistical Physics and Condensed Matter and Others / 40

Analysis of Student Performance in Computer-Based vs. Paper-Based Exams in Introductory Physics

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The use of computer-based exams has become increasingly popular in educational settings due to their potential benefits, such as efficient distribution and grading, immediate feedback, as well as reduced paper usage. However, the effectiveness of computer-based exams in terms of student learning and performance is still a topic of debate. Therefore, this study aims to compare the performance of students in computer-based vs. paper-based exams in introductory physics, and more importantly, understand the factors that affect students' performance. This study will compare the performance of students in computer-based and paper-based exams in introductory physics courses. The data being evaluated is the students' written work on their exams. A physics problem solving rubric by Docktor and Heller will be used to measure the quality of the written work and problem solving. This rubric focuses on the following measures: 1) useful description, 2) physics approach, 3) special application of physics, 4) mathematical procedures, and 5) logical progression. The data will be used to: 1) compare the performance of students in computer-based vs. paper-based exams; 2) analyze the relationship between students' performance and students' background information, such as GPA, SAT score, grade in prerequisite course, whether students are transfer/non-transfer students, major/minor, and the number of times students have taken the course. The study aims to provide insights into the effectiveness of the different exam delivery methods in terms of student learning and performance in introductory physics courses. The results will contribute to understanding of factors affecting student exam performance, which can be used to improve students'experience in the computer-based exam, and to infer possible predictors of students' performance.

Academic year:

5th year and/or beyond

Research Advisor:

Donna Stokes, PhD

Statistical Physics and Condensed Matter and Others / 41

Quantum dynamics of nonequilibrium states in charge density waves

Author: John H. Miller^{None}

Co-authors: Martha Villagran; Johnathan Sanderson; Jarek Wosik

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The charge density wave (CDW) is known to carry electric current en masse, but the transport mechanism remains poorly understood at the microscopic level. Its quantum nature is revealed by several experiments, including h/2e Aharonov-Bohm oscillations in CDW conductance vs. magnetic flux in TaS3 rings. Here we discuss further evidence for quantum transport [1]. We find that, for temperatures ranging from 9 to 474 K, current-voltage plots of three trichalcogenide materials agree almost precisely with a modified Zener-tunneling curve and with time-correlated soliton tunneling model simulations. We treat the Schrödinger equation as an emergent classical equation that describes fluidic Josephson tunneling of paired electrons between emergent nonequilibrium states, such as fluidic soliton and anti-soliton domain walls. An extension of this 'classically robust' quantum picture explains the h/2e magnetoconductance oscillations and switching behavior in CDW rings. We consider potential applications in quantum information processing.

Academic year:

5th year and/or beyond

Research Advisor:

Dr. John H. Miller

Material Science / 42

NiMo based bifunctional catalysts for water electrolysis

Author: Navmi Naik^{None} **Co-author:** Zhigeng Ren ¹

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Seawater electrolysis stands as a promising technology for sustainable hydrogen production and desalination. It consists of two processes, Oxygen Evolution Reaction (OER) and Hydrogen Evolution Reaction (HER). A bifunctional catalyst plays the crucial role of performing both these reactions simultaneously thus reducing the cost of this technology. This study focuses on the synthesis and evaluation of a bifunctional catalyst, NiFe/NiMo. Due to the good HER and OER activity of this catalyst, the AEM electrolyzer exhibited a good performance for water electrolysis, achieving a current density of 1000 mA cm^{-2} at 1.87 V. Further experiments under quasi-industrial conditions (6 M KOH & seawater, 60 °C) showed that a three electrode electrolyzer delivered a current density 1000 mA cm^{-2} at a low voltage of 1.63 V. Stability testing of the electrolyzer showed that it exhibited good durability for over 100h. This work presents a general and economic approach towards the development of a bifunctional catalyst for water electrolysis.

Academic year:

3rd year

Research Advisor:

Dr. Zhifeng Ren

¹ University of Houston

Material Science / 43

Thermoelectric Properties of N type Mg3Bi2-N type Bi2Te3 Composites

Author: JUNAID UR REHMAN^{None}

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This study investigates the thermoelectric properties of Mg_3Bi_2 compounded with varying amounts of Bi_2Te_3 to enhance its thermoelectric performance for cooling applications. The composites were synthesized using a solid-state reaction by ball milling method and characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), and energy-dispersive X-ray spectroscopy (EDS), ZEM 3 and LFA. The thermoelectric properties, including the Seebeck coefficient, electrical conductivity, and thermal conductivity, were measured across a range of temperatures from 300K to 600K. The results reveal that the addition of Bi_2Te_3 to Mg_3Bi_2 leads to significant improvements in thermoelectric performance around 500K. Specifically, the composites exhibit enhanced electrical conductivity and reduced thermal conductivity compared to the pristine Mg_3Bi_2 . Furthermore, the Seebeck coefficient of the composites demonstrates a favorable trend towards increased thermopower. These findings suggest that $Mg_3Bi_2/Bi_2/Te_3$ composites hold promise for efficient thermoelectric cooling applications, offering a potential pathway for advancing solid-state cooling technologies. Further optimization of composite compositions and fabrication techniques may lead to enhanced thermoelectric performance and broader applicability in cooling devices.

Academic year:

3rd year

Research Advisor:

Zhifeng Ren

High Energy and Quantum Field Theory / 45

Particle Production as a Function Transverse Spherocity in pp Collisions at 13 TeV

Author: Jeseleth Van Rose^{None}

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Proton-proton (pp) collisions with high charged-particle multiplicities at the LHC have revealed similar phenomena to the observed in Pb-Pb collisions, where a strongly interacting Quark Gluon Plasma (sQGP) is created. These include the observations of radial and anisotropic flow and the enhanced production of strange particles. Since the mechanisms for hadron production are currently not well understood, particle production is explained using phenomenological models. For example, perturbative Quantum Chromodynamics (pQCD) models based on hard scatterings, such as PYTHIA, describe hadron production via string fragmentations and rope hadronization.

In this contribution, I will show results using the PYTHIA model and how event shape observables like spherocity can help to isolate and study events where particle production is dominated by soft or hard QCD processes. This is done in an effort to pin-point the underlying mechanisms of the collective behaviour observed in pp collisions systems, such as radial flow and long-range angular correlations. Furthermore, published results of charged unidentified particles as a function of spherocity will be shown.

 ${\bf Academic\ year:}$

1st year

Research Advisor:

Dr. Omar and Dr. Bellwied