Polish-German WE-Heraeus Seminar & Max Born Symposium

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Synagoge Görlitz

Book of Abstracts

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Production of charm quarks in hot QCD matter

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We study the production of charm quarks in hot QCD using the effective quasiparticle framework. The evolution of the medium is described by hydrodynamic simulations in 2+1 dimensions, with temperature-dependent shear viscosity taken into account. We compute the number of charm-anticharm pairs with the above setup and juxtapose it to the results acquired for the quark-gluon plasma described as a perfect fluid propagating only longitudinally. We solve the rate equation for the charm quark fugacity and then analyse how number of charm quark depends on the set of different parameters (number of dimensions, viscosity, chemical equilibration of other particles in the system).

Lectures / 2

Dynamically assisted tunneling in the impulse regime

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We investigate how tunneling through a potential barrier, V(x), can be intensified by time-varying electrical fields, whether they take a pulse-shaped form or adhere to harmonic oscillations. To facilitate numerical computations significantly, we employ the Kramers-Henneberger frame. In the context of a periodically driven system, we aim to identify clear resonance signatures when the incident energy E matches the driving frequency, ω=E, revealing the breakdown of the time-averaged potential approximation. Regarding the dependence on a pulse-shaped electrical field, we discover that, in addition to the known effects of pre-acceleration and potential deformation present in the adiabatic regime, there is also energy mixing, reminiscent of the Franz-Keldysh effect in the nonadiabatic (impulse) regime. Specifically, the pulse Ax(t) can enhance tunneling by effectively propelling a portion of the wave function beyond the rear end of the barrier.

For practical experimental applications, especially in solid-state physics, we examine a simplified model utilizing a rectangular potential. This model can also be validated by comparing it with analytical results. Additionally, we explore the truncated Coulomb potential, which holds relevance in the context of nuclear fusion.

Lectures / 3

Sauter-Schwinger Effect for Colliding Laser Pulses

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In ultra-strong electric fields energy can be converted into electrons and positrons. We introduce a novel approach to calculate the mean particle number in collisions of short-pulsed laser fields. In this regard, we further discuss the different regimes of pair production in terms of their unique signatures in particle phase-space and identify the relevant time scales regarding particle formation within and beyond perturbation theory.

Lectures / **4**

Understanding electronic correlations in warm dense quantum plasmas

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Warm dense matter (WDM)—an extreme state that is characterized by extreme densities and temperatures—has emerged as one of the most active frontiers in plasma physics and material science. In nature, WDM occurs in astrophysical objects such as giant planet interiors and brown dwarfs. In addition, WDM is highly important for cutting-edge technological applications such as inertial confinement fusion and the discovery of novel materials. In the laboratory, WDM is studied experimentally in large facilities around the globe, and new techniques have facilitated unprecedented insights. Yet, the interpretation of these experiments requires a reliable diagnostics based on accurate theoretical modeling, which is a notoriously difficult task [1].

In this work, I will give an overview of how we can use exact ab-initio path integral Monte Carlo (PIMC) simulations [2] together with thermal density functional theory (DFT) calculations to get new insights into the behavior of WDM. Moreover, I will show how switching to the imaginary- time representation allows us to significantly improve the interpretation of X-ray Thomson scattering (XRTS) experiments, which are a key diagnostic for WDM [3]. Specifically, I will present a model-free temperature diagnostic [4] based on the well-known principle of detailed balance, but available for all wave numbers, and a new idea to directly extract the electron—electron static structure factor from an XRTS measurement [5]. As an outlook, I will show how new PIMC capabilities will allow to give us novel insights into electronic correlations in warm dense quantum plasmas, leading to unprecedented agreement between experiments [6] and theory.

[1] M. Bonitz et al., Physics of Plasmas 27, 042710 (2020)
[2] M. Böhme et al., Physical Review Letters 129, 066402 (2022)
[3] S. Glenzer and R. Redmer, Reviews of Modern Physics 81, 1625 (2009)
[4] T. Dornheim et al., Nature Communications 13, 7911 (2022)
[5] T. Dornheim et al., arXiv:2305.15305 (submitted)
[6] T. Döppner et al., Nature 618, 270-275 (2023)

Lectures / **5**

Monte-Carlo event generation for the interaction of x-ray laser fields and hot electrons

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With the advent of advanced laser systems producing high-frequency X-ray beams, e.g. the EuropeanXFEL as a prominent example, a regime of laser-plasma interaction is reached, where all-optical methods, as used in particle-in-cell simulations, are no longer applicable. Instead, the interaction of hot electrons and the X-ray laser pulse needs to be modeled with a QED-driven approach. Furthermore, future experiments taking place at HED-HIBEF, LCLS, and other facilities targeting this regime, will encounter processes in x-ray scattering from (laser-driven) relativistic electrons, where the effects of the energy spectrum of the x-ray laser field as well as multi-photon interactions can not be neglected anymore.
To explore this regime, where strong fields meet high frequencies, we present a novel approach for a numerical modeling tool, QED.jl, which inherently uses exact strong-field QED descriptions. This brings, for the first time, the technique of Monte-Carlo event generation to X-ray laser physics experiments.

Lectures / 6

T-Matrix Theory of Quark-Gluon Plasma

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Investigating the properties of the strongly coupled quark-gluon plasma (sQGP) remains a topic of great current interest. In particular, an understanding of how the sQGP's remarkable transport properties, as inferred from experiment, emerge from the underlying QCD interactions is a formidable challenge. In this talk, we will introduce a quantum many-body approach that is aimed at addressing this challenge. Starting from the heavy-flavor sector where the large masses of charm and bottom quarks enable controlled approximations, we self-consistently evaluate the in-medium one- and two-body spectral functions. We discuss how the approach can be constrained by first-principle lattice-QCD calculations and applied to compute transport parameters of heavy quarks and the sQGP, with applications to heavy-ion collisions.

Poster flash talks / 7

Structure prediction of iron hydrides at high pressures with machine-learned interatomic potentials

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Understanding the composition of Earth's core and mantle is a major challenge in geoscience and materials science. The core is primarily made of iron, but its density is known to be slightly lower than pure iron. Hydrogen contributes to this density deficit, leading to significant interest in the properties and structure of iron hydrides under high pressure.

Previous studies have shown that the dhcp phase of FeH remains stable at
lower pressures (10-40 GPa) but undergoes phase transitions to hcp and fcc phases at higher pressures. This study focuses on a theoretical exploration of the potential energy surfaces (PESs) of FeH under varying pressure conditions. The objective is to demonstrate the effectiveness of automated and systematic methods for training and validating transferable machine-learned interatomic potential (ML-IAP) using global
optimization techniques. Utilizing this potential, which significantly reduces computational costs, the phase diagram of the stoichiometric Fe-H system is analyzed across a range of pressures.

To achieve this, we utilize the PyFLAME code to construct a highly transferable ML-IAP. With this accurate potential, the PESs of bulk FeH structures are systematically investigated through global sampling using the minima hopping method. This comprehensive exploration enables the prediction of stable and metastable iron hydrides from 0 to 100 GPa. Density functional theory calculations are conducted to refine the predicted structures and evaluate their dynamical stability.
The findings of this study reveal a wide range of novel low-energy polymorphs of FeH at each pressure level, alongside the recovery of well-known structures in the literature.

Poster flash talks / 8

Physics-Informed Neural Networks as Solvers for the Time-Dependent Schrödinger Equation

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We demonstrate the utility of Physics-Informed Neural Network based solvers for the solution of the Time-Dependent Schrödinger Equation. We study the performance and generalisability of PINN solvers on a simple quantum system. The method developed here can be potentially extended as a surrogate model for Time-Dependent Density Functional Theory, enabling the simulation of large-scale calculations of electron dynamics in matter exposed to strong electromagnetic fields, high temperatures, and pressures.

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Strong phase transitions in neutron star mergers

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The first detection of gravitational waves form a neutron star merger some years ago has highlighted the prospects of inferring properties of high-density matter from these spectacular astrophysical events. In particular, the postmerger phase represents an environment of hot and dense matter implying that the different observables from this phase carry valuable information. We will provide an overview on neutron star mergers and discuss implications from current and future observations for better understanding the properties of high-denisty matter including the possibility of a phase transition to deconfined quark matter.

Lectures / 10

Matter at high energy densities in planetary interiors

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We apply large-scale molecular dynamics simulations based on density functional theory (DFT-MD) to infer the high-pressure phase diagram of hydrogen-helium and H-C-N-O mixtures. Of particular interest is the nonmetal-to-metal transition in dense fluid hydrogen that occurs at few megabars (metallization). Furthermore, demixing of hydrogen and helium is predicted at about the same extreme conditions which leads to helium rain in the deep interior of gas giant planets like Jupiter and Saturn. We calculate the corresponding equation of state data and transport properties like electrical and thermal conductivity and discuss the impact of our results on the interior, evolution, and magnetic field of giant planets like Jupiter and Saturn (H-He), Uranus and Neptune (H-C-N-O mixtures), and corresponding extra-solar planets (e.g. hot Jupiters).

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Physics-enhanced neural networks for equation-of-state calculations

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Fast and accurate equation-of-state (EOS) data is of critical importance in the warm dense matter regime, for example as input to hydrodynamic codes used in inertial confinement fusion modelling. Since EOS data must be generated on-the-fly for many applications, a tabular approach based on interpolation of known data points is generally used. Alternatively, average-atom models are (in some cases) fast enough to generate on-the-fly EOS data in an *ab initio* way, i.e. without empirical inputs. In this presentation, we present a newly-developed method which can be considered a hybrid of these two approaches. In our method, we use data generated by average-atom models as input features to a neural network model [1], which is trained on the first-principles EOS dataset of Militzer *et al.* [2]. This approach has several advantages relative to using an unmodified average-atom model, and also compared to standard interpolation techniques.

[1] Callow, T. J., Kraisler, E., & Cangi, A. (2023). Physics-enhanced neural networks for equation-of-state calculations. arXiv preprint arXiv:2305.06856.
[2] Militzer, B., González-Cataldo, F., Zhang, S., Driver, K. P., & Soubiran, F. (2021). First-principles equation of state database for warm dense matter computation. Phys. Rev. E, 103(1), 013203

Poster flash talks / 12

Impact of pions on binary neutron star mergers

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We investigate the impact of pions on simulations of neutron star mergers and explore their effects on gravitational-wave observables. We model both charged and neutral pions as a non-interacting Boson gas with chosen values of constant effective mass. We incorporate these pions into temperature and composition-dependent equations of state, either as a condensate or a thermal population. Compared to models without pions, we observe changes in the properties of cold, non-rotating neutron stars, including reductions in maximum mass, radius, and tidal deformability. We then conduct several relativistic hydrodynamical simulations of neutron star mergers using these modified equations of state. We find the inclusion of pions in general softens the equation of state, which is particularly pronounced for smaller effective pion masses. We find an increase in the dominant postmerger gravitational-wave frequency by up to 150Hz and a reduction of the threshold binary mass for prompt black-hole formation by up to $0.07M_{\odot}$. We examine empirical relationships that correlate the threshold mass or the dominant postmerger gravitational-wave frequency to the stellar parameters of nonrotating neutron stars. These correlations are formulated to extract these stellar properties from merger observations and are built based on large sets of equation of state models which do not incorporate pions. Comparing these empirical relations with our calculations including pions, we observe that they remain valid to good accuracy and justifies their use despite not accounting for the potential impact of pions. Additionally, we also address the mass ejection by neutron star mergers and observe a moderate enhancement of the ejecta mass by a few ten per cent.

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Correlations and Semi-Universal Relations Connecting Nuclear Matter and Neutron Stars

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The close correspondence between neutron star matter pressure near the saturation density and the radii of typical neutron stars is an example of a semi-universal relation, as is the Yagi-Yunes I-Love relation connecting the moments of inertia and the tidal deformability of neutron stars. These relations are valid for all or nearly all equations of state to high precision. Using an extensive database of hundreds of Skyrme- and RMF-type nuclear interactions proposed over the last several decades, I will demonstrate several additional relations that could prove valuable in interpreting astronomical observations of neutron stars. For example, the central energy density and pressure of the maximum mass star are highly correlated with the maximum mass, the radius of the maximum mass star, and the radius of the star with half the maximum mass. Other relations can be found that are able to predict the central energy density and the pressure of smaller mass stars using mass-radius information only. Such relations may allow the semi-analytic inversion of the mass-radius diagram.

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Strong field Quantum Electrodynamics: from amplitudes to physical effects

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The presentation will begin with a concise introduction to Quantum Electrodynamics (QED) in the presence of external background fields, offering insights into the fundamental interactions between matter and electromagnetic fields. Following this, we will delve into the significance of light-by-light scattering in QED, examining ist amplitude (also known as the four-photon amplitude) with general kinematics. We will highlight its applications in accurately measured quantities, such as the electron's magnetic moment and the Lamb shift observed in atomic energy levels. Furthermore, we will explore the remarkable phenomena associated with light-by-light scattering, notably vacuum birefringence. Despite its long-standing prediction, experimental observation of this phenomenon remains challenging due to its tiny effects. We will provide an overview of the theoretical foundations behind vacuum birefringence and present our proposed experimental approaches and ongoing progress in this intriguing research area.

Lectures / 15

Elasticty, geometry and fractons

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This seminar explores the evolving field of fractons, quasiparticles with limited mobility, and their relationship with elasticity. Mechanical properties of crystals on curved substrates mix elastic, geometric and topological degrees of freedom. In order to elucidate properties of such crystals I formulate the low-energy effective action that combines metric degrees of freedom with displacement fields and defects. I propose new dualities for elasticity coupled to curved geometry formulated in terms of tensor gauge theories. I show that the metric degrees of freedom, evolving akin to linearized gravity are mapped to tensors with three indices. Finally, when coupled to crystals, metric degrees of freedom become gapped and, in the presence of dislocations and disclinations, multivalued. The elastic degrees of freedom remain gapless and mapped to symmetric gauge fields with two indices. In analogy with elasticity on flat space we assume that the trace of the total quadrupole moment is conserved. In the dual formulation, topological defects, which act as sources for the gauge fields, are fractons or excitations with restricted mobility. This leads to generalized glide constraints that restrict both displacement and gravitational defects.

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Many photons (under extreme conditions): light-by-light scattering

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In the theory of Quantum Electrodynamics, loop corrections induce nonlinear interactions for the electromagnetic fields, allowing for effects such as light-by-light scattering.
One of the most promising scenarios for its experimental detection regards the quantum vacuum diffraction and birefringence of x-rays at the combined field of two optical lasers.
Reviewing this framework, we will compare various proposed scenarios; as a way to deal with experimental constraints, we analyze cases in which the initial and final x-ray photons differ not just in polarization, but also in propagation direction or energy. Based on arxiv:2208.14215 .

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Equation of State and composition of compact stars with hyperons and Delta-resonances: Three-dimensional tables

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The equation of state (EoS) and composition of Δ-resonance admixed hypernuclear, neutrino-trapped matter is studied over a wide range of baryon densities, temperatures and electron fractions, covering the characteristic conditions encountered in neutron star binary merger remnants and supernovas.We adopt the covariant density functional (CDF) formalism, adjusting it appropriately to include the full $J^P = 1/2^+$ baryon octet as well as the non-strange members of $J^P = 3/2^+$ decuplet. The density-dependent coupling parameters have been selected according to the existing laboratory and astrophysical data. The emergence of Δ-resonances at finite temperatures is found to result in a softer EoS of hypernuclear matter at intermediate densities and a stiffer one at high densities. Moreover, at higher temperatures the softening effect due to the hyperons and Δ particles becomes more distinct. An additional consequence of increased temperature is that for all the particles of the baryon octet and the non-strange resonances included in our models, their respective onset baryon density decreases. Finally, it is noteworthy that the presence of hyperons and Δ-resonances at temperatures associated to supernovas and binary neutron star merger events could be capable of leaving a traceable implication on the neutrino signal emitted during these astrophysical phenomena.

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Probing hadron-quark phase transition in twin stars using f-modes

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Although it is conjectured that a phase transition from hadronic to deconfined quark matter is possible in the ultrahigh density environment in Neutron Stars, the nature of such a transition is still unknown. Depending on whether there is a sharp or slow phase transition, one may expect a third family of stable compact stars or "twin stars" to appear, with the same mass but different radii compared to Neutron stars. The possibility of identifying twin stars using astrophysical observations has been a subject of interest, which has gained further momentum with the recent detection of gravitational waves from binary neutron stars. In this work, we investigate for the first time the prospect of probing the nature of hadron-quark phase transition with future detection of gravitational waves from unstable fundamental (f-) mode oscillations in Neutron Stars. By employing a recently developed model that parametrizes the nature of the hadron-quark phase transition via "pasta phases",

we calculate f-mode characteristics within a full general relativistic formalism. We then recover the stellar properties from the detected mode parameters using Universal Relations in GW asteroseismology. Our investigations suggest that the detection of gravitational waves emanating from the f-modes with the third-generation gravitational wave detectors offers a promising scenario for confirming the existence of the twin stars. We also estimate the various uncertainties associated with the determination of the mode parameters and conclude that these uncertainties make the situation more challenging to identify the nature of the hadron-quark phase transition.

Poster flash talks / 19

Towards an effective model of neutron star crust: dynamics of impurity in superfluid neutron matter

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Among numerous challenges in astrophysics, construction of effective model of neutron star crust seems to be particularly interesting. The inner crust is supposed to consist of proton impurities immersed in the superfluid neutron matter –one can examine such system with time-dependent numerical simulations, which can be proceeded with recently developed W-BSK Toolkit based on Brussels-Montreal Skyrme (BSk) density
functional. This kind of calculations requires high accuracy and computational power, therefore, integral part of these studies isHigh-Performance Computing. One of the crucial properties of the impurities is their effective mass, which can be extracted from the results
of these simulations; moreover, they allow to study other mechanisms of dissipation, such as Cooper pair breaking and creation of quantum vortices. Obtained results can give significant contribution to the studies concerning the model of neutron star crust.

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Towards microscopic simulator of neutron star crust: merging progress in fields of ultracold atomic gases and nuclear physics.

Author: Gabriel Wlazłowski[None]

The density functional theory (DFT) is one of physics's most popular methods for simulating systems' microscopic properties. It allows for studies of many-body Fermi systems' static, dynamic, and thermodynamic properties in a unified framework while keeping the numerical cost at the same level as the mean-field approach. The development of (super)computing techniques in the last decade allows for DFT approaches to track the microscopic dynamics of systems consisting of tens of thousands of particles. This progress is supported by the construction of local energy density functionals of high accuracy for strongly interacting Fermi systems, which also include pairing
(superfluid) correlations. In this seminar, I will discuss possibilities that emerge from joint progress in the fields of nuclear and ultracold Fermi gas physics, and high-performance computing in the context of the construction of general-purpose tools for the modeling of neutron star crust. I will focus on the issue of modeling arbitrary phenomena taking place on scales exceeding Wigner-Seit cell size, with protons and neutrons as dynamical degrees of freedom.

Lectures / 21

Thermodynamics of QCD with quarks and multi-quark clusters

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We present a generalized Beth-Uhlenbeck approach to thermodynamics of QCD, which treats hadrons as color singlet multiquark clusters in medium with a background gluon field coupled to the underlying chiral quark dynamics. Colored multiquark clusters are treated on the same footing. The confining aspect of QCD is modeled by the property of color SU(3) center symmetry within the Polyakov gauge and by a large vacuum quark mass motivated by a confining density functional approach. The spectrum of multiquark clusters consists of a bound and a scattering continuum states. For the corresponding cluster-cluster phase shifts we discuss simple ansätze that capture the Mott dissociation of multiquark clusters. This allows us to demonstrate the role of the continuum correlations and introduce an improved model that includes them in a generic form. We calculate thermodynamic properties such as baryon density and entropy and compare them to the results of lattice QCD. A striking result is the suppression of the abundance of colored multiquark clusters at low temperatures by the coupling to the Polyakov loop and their importance for a quantitative description of lattice QCD thermodynamics at non-vanishing baryochemical potentials. We demonstrate that the limits of a hadron resonance gas at low temperatures and perturbative QCD at high temperatures are correctly reproduced. A comparison with lattice calculations shows that the model provides a unified and systematic description of the properties of the quark-gluon-hadron system.

Lectures / **23**

The global CREDO cosmic radiation research project and the synergy of its extensive scientific research and popularization activities

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The CREDO scientific project was established in 2018 to create networks
of detectors across the Earth to record cosmic radiation. This network is being created very dynamically (several million particle registrations so far) and its main purpose is to detect correlations between atmospheric showers in different parts of the Earth, i.e. to study primary cosmic radiation showers arising far outside the Earth's atmosphere. Scientific conclusions from the registration of such showers concern dark matter, superheavy particles outside the Standard Model and the quantum structure of space. A very recent CREDO observation is the correlation between global cosmic ray recordings
and Earth's global seismic activity. All these goals and initial results are the first to be launched on Earth on such a large scale and with such great determination. The motivation of this presentation is to familiarize you with the goals and current activities of CREDO and to encourage you to participate widely on many levels: from collecting data, through their analysis, to drawing scientific conclusions.

Lectures / **24**

Kinetic equation approach to pair creation in strong fields

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Experimental validation of the Schwinger effect i.e. particle production from QED vacuum, remains elusive. State-of-the-art facilities are yet to generate the required electric field, which is constrained by the electron mass. However, graphene, a 2D condensed matter system with hexagonal lattice structure, behaves like massless Dirac fields near Dirac points. The advantage of this masslessness is the reduced electric field needed to observe Schwinger type particle-hole production. In this presentation I will present a kinetic equation approach to describe such phenomena. The model is capable of producing experimentally observed particle hole creation rate as well as describing the momentum profile of produced particles for various incident electric field pulses.

Lectures / **25**

Hydrodynamic simulations of superdense fluid evolution in heavy-ion collisions

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In extremely hot and dense circumstances nuclear matter no longer consists of neutrons and protons, but of individual quarks and gluons. On Earth, such a state of matter - quark-gluon plasma - can be reached in collisions of heavy nuclei at large energies. However, the expansion and cooling of this matter cannot be described by first-principles calculations, but phenomenological models must be used.

One approach is to model the quark-gluon plasma as a fluid. I will describe the physics of heavy-ion collisions, and the fluid-dynamical models used to describe them.

Poster flash talks / **26**

Strange Matter from the Phenomenology of Neutron Stars and Hypernuclei

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The standard model of fundamental particles has revealed the existence of particles that we were less familiar with and their appearance needs extreme conditions of density and temperature. The most compacted matter on the earth is found in heavy nuclei which can be studied in heavy-ion collision (HIC) experiments. These high densities are interesting to investigate because exotic forms of matter and particles with one or two strange quarks can potentially appear while they are not found in ordinary matter. Therefore, the standard model, by proposing a surprising quantum number, strangeness, made it possible for us to have other states of the hadron classification called hyperons that open new windows for our understanding of matter at higher energy. Recent astrophysical observations have shown us signatures for the appearance of hyperon in the core of Neutron Stars (NS)s, which are the only natural laboratory for such extreme conditions. In the core of NS, not only the appearance of substantial amounts of hyperons is expected but also there is evidence for the appearance of strange quark matter accompanied by a phase transition from hadronic to deconfined quark matter when the density increases. Using experimental data from HIC, more accurate information for hyperons will be provided. Those data will be employed in many-body approaches to obtain the equation of state (EoS) of hypernuclear matter. Microscopic calculations of the EoS of dense matter profoundly affect our understanding of the origin and the thermodynamic properties of matter. I will present my results based on constructing the EoS for hypernuclear matter and will discuss some roles played by hyperons in hypernuclear Physics.

Lectures / **27**

Probing the Quantum Vacuum at the High-Intensity Frontier

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In contrast to many highest-precision tests of Quantum electrodynamics (QED) in low-energy experiments, the high-intensity frontier has remained largely unexplored in the laboratory so far. Ultra-intense lasers coming online these days and in the near future have the potential to discover the nonlinear response of the ground state of nature - the quantum vacuum - to macroscopically controlled strong fields for the first time. I review basic properties of the quantum vacuum based on the Heisenberg-Euler effective theory and report about current efforts towards discovery experiments.
In a second part, I present a novel theoretical exploration of the strong-field limit of QED. Using the functional renormalization group, indications for the the existence of a global solution to the RG equations are provided. The solution corresponds to a fixed function, analogous to a multi-dimensional fixed point, with a strong-field limit being governed by the anomalous dimension of the photon field. The solution is stable on all scales as long as the electric field components remain subcritical.

Poster flash talks / **28**

Material Specific Exchange-Correlation Kernel Across Jacob's Ladder and Temperature Regimes

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We developed a new method [1] that allows one to compute material specific static exchange-correlation (XC) kernel across temperature regimes using standard DFT codes and for any XC functional available in Libxc. We show the results of the static exchange-correlation kernel analysis using various XC functionals for dense electron gas and warm dense hydrogen. By comparing the data to the exact QMC results, we are able to understand the effect of thermal excitations and density inhomogeneity on the exchange-correlation kernel. Moreover, we discuss the results of the analysis of the accuracy of the commonly used XC functionals for warm dense matter simulations [2-6]. The analysis is performed by comparing path-integral quantum Monte-Carlo (QMC) data with KS-DFT results. The application of this methodology for linear response time-dependent DFT calculations is discussed as well [7,8].

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Lectures / **29**

Quantum Monte Carlo and Machine Learning Calculations for matter under extreme conditions

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Dense hydrogen is important because of its ubiquitous presence in the universe, its technological applications and its suitability for developing and testing ab initio simulation methods. Even though it is the "holy grail"of high pressure research, its phase diagram above 100 GPa is uncertain. We have made a new study of its phase diagram using a machine-learned interatomic potential trained with Quantum Monte Carlo (QMC) forces and energies and we find two new stable phases. The high temperature phase has a reentrant melting line with a maximum at higher temperatures (1450K at 150GPa) than previously estimated.

Because continuum QMC methods such as DMC and PIMC are directly formulated in coordinate space, they do not have the limitation of a basis set which helps in disordered systems such as those liquids, chemical reactions, solids with large amplitude motions, and surfaces. Slater-Jastrow-backflow wavefunctions are a compact, efficient and understandable description of systems with strong correlation. An important application for QMC is to provide unbiased data for bespoke force-fields; they have advantages over other accurate electronic structure methods such as those based on DFT. [See Phys. Rev. Lett. 130, 076102 (2023) and arXiv:2310.15994]

Lectures / 30

Cluster-virial expansions for correlated matter

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The properties of strongly interacting Fermi systems are influenced by the formation of bound states. The mass-action law applies in the low density range. At a fixed temperature, a Fermi liquid consisting of quasiparticles is obtained at high density. A phase transition can occur in between. Analytical approaches such as the Matsubara-Green function method are based on perturbation theory and only provide accurate results in some limiting cases, e.g. in the case of virial expansions. The Beth-Uhlenbeck equation for the second virial coefficient is discussed and generalisations, for instance the cluster-Beth-Uhlenbeck equation, are considered. Numerical approaches such as density functional theory or path-integral Monte Carlo simulations provide results for strongly interacting systems that go beyond perturbation theory. Examples are strongly coupled Coulomb systems, especially warm dense matter, and nuclear systems, especially in nuclear reactions and in astrophysics. We discuss the thermodynamic properties of the homogeneous electron gas and transport processes in hydrogen plasmas. For nuclear matter, the composition, the Pauli blocking effect, properties of nuclei and applications in astrophysics are discussed.

Poster flash talks / 31

Impact of vortices on heat capacity in the crust of a neutron star

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Bardeen–Cooper–Schrieffer theory explains how the heat capacity of a superfluid vanishes as the temperature approaches zero. Various mechanisms may suppress the pairing gap in the superfluid, leading to an increased heat capacity. Consequently, this alteration may impact the cooling rate and thermal evolution of neutron stars. The presence of a vortex in superfluid neutron matter adds extra degrees of freedom in which energy is stored, thus contributing to the heat capacity.

Through fully microscopic simulations employing the Superfluid Local Density Approximation (SLDA), it is possible to calculate the finite-temperature energy of the system. We utilize the BSk type energy density functional, a highly accurate nuclear functional designed to align with existing astrophysical constraints. Utilizing this state-of-the-art functional, we estimate the change in the heat capacity resulting from the mere existence of a vortex in the system.

Lectures / **32**

Impact of Multiple Phase Transitions in Dense QCD on Compact Stars

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This talk covers several recent developments in the physics of dense QCD with an emphasis on the impact of multiple phase transitions on astrophysical manifestations of compact stars. It is conjectured that pair-correlated quark matter in β-equilibrium is within the same universality class as spin-imbalanced cold atoms and the isospin asymmetrical nucleonic matter. This then implies the emergence of phases with broken space symmetries and tri-critical (Lifshitz) points. We construct an equation of state (EoS) that extends the two-phase EoS of dense quark matter within the constant speed of sound parameterization by adding a conformal fluid with a speed of sound c_conf=1/√3 at densities ≥10 n_sat, where nsat is the saturation density. With this input, we construct static, spherically symmetrical compact hybrid stars in the mass-radius diagram, recover such features as the twins and triplets, and show that the transition to conformal fluid leads to the spiraling-in of the tracks in this diagram. Stars on the spirals are classically unstable with respect to the radial oscillations but can be stabilized if the conversion timescale between quark and nucleonic phases at their interface is larger than the oscillation period. Finally, we review the impact of a transition from high-temperature gapped to low-temperature gapless two-flavor phase on the thermal evolution of hybrid stars.

Lectures / **33**

Is Dark Matter made up of Primordial Black Holes?

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The cosmic X-ray background radiation has been almost completely resolved into discrete objects, mainly from the growth of massive black holes in the universe. However, a few years ago, evidence for a new population of black holes from the early universe emerged from the correlation of fluctuations in the X-ray and infrared backgrounds. Similarly, quasars have been discovered with astonishingly massive black holes already formed shortly after the Big Bang. The detection of gravitational waves from the merger of pairs of very heavy, apparently non-rotating stellar black holes presents another puzzle. Recently, using the micro-lensing effect and distance determination with the ESA satellite GAIA, about 20 black holes in our galaxy have been discovered with masses that cannot be generated by stellar processes. In the past few months, the discovery of several galaxies that formed very early in the universe with the James Webb Space Telescope has been surprising, seeming to contradict the classical understanding of cosmology. All of these phenomena can be explained by so-called primordial black holes that formed immediately after the Big Bang and may represent the previously unexplained dark matter. In this talk I will in particular focus on the QCD transition in the early Universe.

Lectures / 34

Scalable machine learning for predicting the electronic structure in many-particle systems

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In this presentation, I will present our recent progress in integrating machine learning to significantly boost the computational efficiency of electronic structure calculations [1]. I will specifically address our efforts to speed up density functional theory calculations, for which we have developed the Materials Learning Algorithms framework [2]. Our findings illustrate significant improvements in calculation speed for metals at their melting point. Additionally, our use of automated machine learning has yielded significant reductions in computational resources required to identify optimal neural network architectures, laying the groundwork for extensive investigations [3]. Furthermore, I will show the transferability of our ML model across temperatures [4]. Most importantly, I will present our latest breakthrough, which enables fast neural-network driven electronic structure calculations for systems unattainable by conventional density functional theory calculations [5].

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Lectures / 35

Predictive modeling of experiments on matter under extreme conditions

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Co-authors: Alexander Debus [2]; Anna Willmann ; Attila Cangi [3]; Brian Edward Marre [4]; Finn-Ole Carstens [5]; Franz Poeschel [6]; Jan Vorberger [1]; Jeffrey Kelling [1]; Klaus Steiniger [7]; Pawel Ordyna ; Rene Widera [8]; Thomas Kluge [1]; Tobias Dornheim [9]; Uwe Hernandez Acosta [10]

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High power lasers and X-ray free electron lasers enable experiments on matter under extreme conditions at atomistic resolutions. A singfle high power laser impinging on a solid density target creates a plasma spanning orders of magnitude in density and temperature.

In this talk we present a view on how better physics modeling and understanding can be combined with Exascale computing and machine learning to create a research program integrating experimental discovery with predictive modeling.

Lectures / **36**

Imaging the quark and gluon substructure of the pion

Author: Minghui Ding[1]

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As the theory of quantum chromodynamics has unfolded, the pion has come to be understood as Nature's most fundamental Nambu-Goldstone boson. It is attached to chiral symmetry, which is dynamically broken, quite probably as a corollary of emergence of hadron mass that has measurable implications for the quark and gluon substructure of the pion. Continuum Schwinger function methods are well suited to tackling the pion.
This presentation describes the theoretical developments on pion structure, thereby providing challenges and opportunities for modern and anticipated high-luminosity, high-energy facilities - JLab at 22GeV, the AMBER project at CERN, and electron ion colliders in the USA and China - and surveys the developments in global phenomenological fits and lattice regularised QCD, enabling the picture of the pion to be drawn.

Poster flash talks / **37**

Nuclear clusters and chemical freeze-out in heavy-ion coll.

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Cluster formation is an important signature to investigate the properties of hot and dense nuclear matter. The concept of chemical freeze-out can be used to explain the distribution of clusters, for instance from heavy-ion collisions. The primordial distribution is characterized by the thermodynamic properties of matter at freeze-out and evolves to the observed cluster yields. We discuss medium effects on light cluster production in the QCD phase diagram within a generalized Beth-Uhlenbeck (GBU) approach. In particular, cluster abundances are suppressed at high densities, and are dissolved at the Mott conditions. We investigate the momentum dependence of the Pauli blocking and relate the corresponding Mott lines to those for chemical freeze-out.

Poster flash talks / **38**

Phenomenology of Identified Particle Spectra in Heavy-Ion Collisions at LHC Energies

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The Zubarev approach of the non-equilibrium statistical operator [1] is used to develop a thermal particle generator that can account for the enhancement of the low-pT part of pion spectra by introducing an effective pion chemical potential. This is an alternative to the explanation of the low-pT enhancement by resonance decays. Bayesian inference methods are applied for these scenarios to find the most probable sets of thermodynamic parameters at the freeze-out hypersurface for the case of the transverse momentum spectra of identified particles measured by the ALICE Collaboration [2]. The Bayes factor is determined for these scenarios. The advantages and limitations of the Zubarev approach are discussed.
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[2] B. Dönigus et al., Phys. Rev. C 106, 044908 (2022)

Lectures / **39**

Modeling of transient, non-equilibrium plasma dynamics under extreme conditions –From theory to experiment

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Lectures / **40**

Matter at high energy densities in planetary interiors

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Predictive modeling of of experiments on matter under extreme conditions

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Understanding electronic correlations in warm, dense quantum plasmas

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Scalable machine learning for predicting the electronic structure in many-particle systems

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Cluster virial expansions for correlated matter

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Hydrodynamic simulations of superdense fluids

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T-Matrix Theory of the Quark-Gluon-Plasma

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Thermodynamics of QCD with quarks and multi-quark clusters

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The global CREDO cosmic radiation research project and the synergy of its extensive scientific research and popularization activities

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Probing hadron-quark phase transition in twin stars using f-modes

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Strong phase transitions in neutron star mergers

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Physics-enhanced neural networks for EoS calculations

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Quantum Monte Carlo and Machine Learning Calculations for matter under extreme conditions

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Strong phase transitions in neutron star mergers

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The QCD phase diagram at low temperatures

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Ultracold atomic gases, neutron stars, and nuclei from the perspective of density functional theory

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Elasticity, geometry and fractons

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Correlations and semi-universal relations connecting nuclear matter and neutron stars

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Primordial black holes and QCD transition in Cosmology

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About the WE-Heraeus Foundation

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Probing the Quantum Vacuum at the High-Intensity Frontier

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Monte-Carlo event generation for the interacxtion of x-ray laser fields and hot electrons

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Strong field Quantum Electrodynamics from amplitudes to physical effects

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Sauter-Schwinger effect for colliding laser pulses

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Kinetic equation approach to pair creation in strong fields

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Dynamically assisted tunneling in the impulse regime

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Imaging the quark and gluon substructure of the pion

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As the theory of quantum chromodynamics has unfolded, the pion has come to be understood as Nature's most fundamental Nambu-Goldstone boson. It is attached to chiral symmetry, which is dynamically broken, quite probably as a corollary of emergence of hadron mass that has measurable implications for the quark and gluon substructure of the pion. Continuum Schwinger function methods are well suited to tackling the pion.
This presentation describes the theoretical developments on pion structure, thereby providing challenges and opportunities for modern and anticipated high-luminosity, high-energy facilities - JLab at

22GeV, the AMBER project at CERN, and electron ion colliders in the USA and China - and surveys the developments in global phenomenological fits and lattice regularised QCD, enabling the picture of the pion to be drawn.

Poster flash talks / 67

The Mass and Possible Quantum Numers of X(6900)

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The X(6900) is the first discovered all-charm tetraquark candidate with yet unknown structure and quantum numbers and unusual properties. Results from heavy-ion collision experiments in which the structure X(6900) was discovered by LHCb are compared with results of similar experiments in which the same structure was observed. Possible structures and quantum numbers were determined by solving the Schrödinger equation with Runge-Kutta method and fitting the parameter set of the Fermi-Breit Hamiltonian.

Lectures / 68

Simulations of massive star explosions driven by a first-order QCD phase transition. Neutrino signal and gravitational wave mode analysis

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Astrophysical simulations are crucial for investigating high baryon density environments and exploring the occurrence of a first-order QCD hadron-quark matter phase transition under extreme conditions. Specifically, multi-messenger neutrino and gravitational wave emissions from corecollapse supernovae not only provide a measurable signal for the presence of deconfined quark matter, but also offers insights into the state of matter at extreme conditions within the supernova core [1,2]. This phenomenon manifests as a non-standard second neutrino burst dominated by electron-antineutrinos as well as heavy lepton flavour (anti)neutrinos. Extensive simulations of core-collapse supernovae have been conducted, integrating various stellar progenitor models and equations of state that incorporate the quark-hadron phase transition based on the String-Flip model for deconfined quark matter featuring the relativistic density functional approach [3]. The supernova simulations employ general relativistic neutrino-radiation hydrodynamics with threeflavour Boltzmann neutrino transport, establishing a direct connection between intrinsic signatures of the neutrino signal and selected bulk properties of the hadron-quark hybrid equation of state. Notably, a set of novel empirical relations has been discovered, potentially providing constraints on the onset density of a phase transition [4]. This determination is presently one of the major
uncertainties in contemporary investigations of the QCD phase diagram, and it can be informed by future neutrino observations of the next galactic core-collapse supernova.

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Simulations of massive star explosions driven by a first-order QCD phase transition. Neutrino signal and gravitational wave mode analysis

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Poster flash talks / 70

An Invariant of the xTB initial Hamiltonian as a chemical Descriptor for DFT regression

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We show that the first-guess electronic Hamiltonian from xTB (extended tight-binding) calculations can be used as a chemical descriptor with all common invariances (i.e. translation, rotation, reflection, and permutation) via simple orthonormal matrix transformations. Artificial neural networks (ANNs) were trained on a labeled dataset of water dimer clusters with the aforementioned first-guess Hamiltonian matrices as inputs to evaluate their potential as descriptors for a regression of the converged SCF Hamiltonian and the corresponding electron density. Our tests using linear regression resulted in a band-structure energy mean absolute error of 15.02 mHa with our invariances applied compared to 73.58 mHa without the invariances.