Fusion Energy Sciences
Quantum Information Science Awards Abstracts

High Energy Density Quantum Matter

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We will explore a new realm of quantum behavior at high-energy-density (HED) conditions *to understand and realize extremes of quantum matter behavior, properties, and phenomena.* Since the earliest days of quantum mechanics, the realm of quantum matter has been limited to low temperatures, restricting the breadth of quantum phenomena exploited and explored. This work will tune the energy density of matter into a high-energy-density quantum regime. Quantum behavior often emerges, for example, when the De Broglie wavelength, $\lambda_{\mathrm{deBroglie}}$, becomes comparable to the interatomic distance α_{nn}. Thus, usually the temperature and mass are reduced to sufficiently increase $\lambda_{\mathrm{deBroglie}}$. This project however will take advantage of new developments in HED science which enable the controlled manipulation of pressure, temperature, and composition, (*P-T-X*), opening the way to revolutionary quantum states of matter. Compression experiments can now tune $\alpha_{\mathrm{nn}} < \lambda_{\mathrm{deBroglie}}$, bringing the quantum behavior of matter to unprecedentedly high temperatures, and even bringing $\alpha_{\mathrm{nn} <} a_{\mathrm{Bohr}}$, breaking foundational building blocks of quantum mechanics and transferring the quantum behavior to the macroscale.

Controlled Mbar (100 GPa or one million atmospheres) to Gbar (100 TPa or one billion atmospheres) pressure can produce up to 1000-fold compression of materials, providing precise control of interatomic distances and therefore quantum orbitals and their energies. Exploiting this capability, our research holds the potential for creating altogether new states of matter including “hot” superconductors, designer topological insulators, and insulating plasmas, thereby advancing our understanding of quantum systems. Such quantum states of matter, forged in the crucible of atomic-scale-pressures, is a rich opportunity for HED science that will help lay the foundation for a new field of HED quantum extremes.

Recent experiments and theory are at the incipient conditions to those now accessible, but are still rich with discovery, including an observed new class of hydrogen-rich superconductors with critical temperatures above 260 K, predicted superconductors with even much higher critical temperatures combined superconducting-superfluid states, exotic chemical bonding, electride insulators characterized by interstitial electron loc alization, and new topological materials.

Our effort is broken down into four technical thrusts. Thrust 1 involves theoretical and experimental work and will explore novel quantum structures to near the TPa regime (0.5TPa or 5 Mbar) such as electrides, topological materials, superconductors, bonding rules versus energy density, and kinetic pathways to metastable structures. Thrust 2 will explore a new generation of HED hot superconducting behavior in hydrogen-rich systems to ~0.5 TPa. Binary and ternary hydrides and pure hydrogen (superconducting) systems will be explored. Thrust 3 will extend Thrusts 1 and 2 to much higher energy density—the atomic-scale-pressure regime (TPa regime). Thrust 4 will develop new techniques to explore both the structural complexity and exotic electronic behavior of matter and materials in the three other Thrusts.

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Quantum Leap for Fusion Energy Sciences

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Quantum information science (QIS) holds the promise to deliver large gains in measurement sensitivity, information processing, and computing power and could represent a paradigm shift for realizing the mission of the Fusion Energy Sciences (FES) program "to bring a star to earth." This project will develop fundamental understanding of how to use emerging quantum computing capabilities to accelerate applications of interest to the FES program by proceeding along two thrusts. The first thrust will develop conceptual approaches to FES-relevant quantum algorithms that will be useful in the long term with error correction. We will work to (1) understand how future quantum algorithms can provide game-changing capabilities for FES applications that rely on both classical and quantum simulation, (2) understand how a quantum co-processor with limited capabilities could potentially be used to accelerate key algorithmic steps used within FES applications, and (3) develop a set of FES-inspired model problems suitable for implementation on near-term quantum computing hardware that can address challenging topics such as the "continuum lowering problem," an important unsolved quantum many-body problem in the physics of plasmas. The second thrust will implement specific quantum algorithms on present-day quantum computing platforms without active error correction. We will (1) perform the first quantum calculations of FES-inspired dynamical systems, (2) demonstrate the ability of present-day quantum computing hardware to simulate both integrable and chaotic dynamical systems of interest to FES, and (3) demonstrate the first use of quantum optimization algorithms to find the fastest growing plasma instability. Specific implementations will be developed for the "Quantum Design and Integration Testbed" (QuDIT) computing facility onsite at LLNL as well as user facilities that are available through the ASCR "Quantum Testbeds for Science" program and through commercial platforms. The results and performance of the quantum computations will be compared to theoretical models of algorithm and hardware performance.

The goal of this project is to explore the promise that quantum computing has to offer, which, if realized, has the potential to accelerate progress toward achieving the goals and objectives of FES. The project will focus on solving concrete model problems in order to gain the expertise necessary to eventually develop quantum solutions for realistic FES applications. The necessary concepts will be developed by a cross-cutting collaboration of experts in plasma physics, high energy density physics, quantum simulation, and quantum computing who understand both the needs of FES and the benefits and challenges of quantum computing. There is great potential for the discovery of innovative ideas to ultimately have a transformative impact on the mission of "bringing a star to earth."

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Quantum Computing for Fusion Energy Materials

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General Atomics and Argonne Leadership Computing Facility have come together to carry out a collaborative project with the objective of demonstrating that fusion relevant chemistry and materials science phenomena can be accurately formulated for near-term quantum computing hardware. As quantum computing technology rapidly advances, these investigations will have a transformative effect on the understanding of fusion materials for the long-term. The plasma-materials interface is a targeted research direction for FES, including engineered materials for tritium control and the understanding of plasma facing surfaces in reactor-relevant conditions. A near-term material of interest is beryllium, which has been selected for use as a first wall cladding in the ITER tokamak. However, important questions remain regarding beryllium surface chemistry and the severity of deuterium and tritium sequestering.

This project formulates quantum chemistry techniques for beryllium and beryllium hydrides into quantum computation circuits (gate models), validates their performance relative to known classical methods, and evaluates their quantum hardware resource usage and resilience to hardware noise. Advanced techniques are required to correctly simulate the electronic structure of materials in the severe fusion plasma environment. The techniques under investigation here include utilizing extended basis sets, evaluating time-dependent Hamiltonians by including electromagnetic radiation, a hybrid quantum- classical approach to simulating nonequilibrium dynamics, and a novel approach to preparing excited states.

Although the availability of extended bases (orbitals) and excited states plays a crucial role during the bond formation and breaking processes – for example, to correctly predict chemical reaction rates – they have not yet been widely explored for quantum computation. This project bridges the knowledge gap by creating various representations of extended bases and evaluating them for their resource demands in terms of the number of qubits that are required to encode the problem, the number of quantum (logic) gate operations that must be performed, and the fidelity of the gate operations that must be obtained in order to overcome the effects of noise. The feasibility of simulating larger molecules and higher Z materials is examined by using effective core potentials to approximate the core electrons of larger systems. This project also extends the forefront of molecular dynamics on quantum computers with two methods: by direct evolution of a time-dependent Hamiltonian using a Suzuki-Trotter discretization, and through a hybrid approach employing classical evolution of quantum forcing that is capable of ab initio nonequilibrium dynamics.

Furthermore, this project seizes on the current opportunity by which the quantum formulation of these phenomena for very small molecules may be verified using classical computers as emulators and through established methods. The long-term challenge is that these simulations do not scale in a way that is amenable to classical computation at the hardware level, and that is where quantum computers, and the algorithms that run on them, are poised to take us beyond what is currently possible on classical hardware towards understanding and engineering fusion energy materials.

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Quantum algorithms for fusion-plasma dynamics

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The dynamics of fusion plasmas – and, more generally, that of many space and astrophysical plasmas – is governed by nonlinear partial differential equations whose numerical solution presents a tremendous computational challenge even in the most advanced supercomputing platforms in existence today. Quantum information science offers an opportunity to develop algorithms for solving problems faster than classical computers. In several areas such as optimization and simulation, such algorithms are expected to offer dramatic speedups over their classical counterparts. Of particular interest to the simulation of fusion plasmas are the already existing quantum algorithms for matrix inversion, fast Fourier transform, and polynomial root finding. This work aims to explore these algorithms, and possibly develop novel ones, that will enable the solution of nonlinear partial differential equations relevant to fusion-plasma physics on existing and near-term quantum computers. The research that we are carrying out generally consists of: devising the physical formulation of the problem, and the numerical algorithm, that are most suitable for quantum computation; followed by the derivation of the quantum algorithm and, lastly, its actual implementation on a quantum machine, utilizing expertise and infrastructure at BBN Technologies. We remark that while our choice of problems to tackle is driven by their application to magnetic confinement fusion, the techniques that we are developing will be useful to a wide variety of plasma physics problems, and beyond: the types of nonlinearities that appear in plasma equations are common to many other fields of physics. Our team combines experts from theoretical and computational plasma and fusion physics and from both theoretical and applied aspects of quantum computing and quantum information sciences.

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Plasma Theory Connections to Quantum Information

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The research program includes: 1) Development of first-principle simulations of ultra-cold ion plasmas used for quantum information research; and 2) development of quantum algorithms for solving computational plasma kinetic theory. Fusion plasma science has a long history and culture where large-scale nonlinear kinetic simulation is routine and brings this experience to direct numerical simulation of ultra-cold ion plasmas used for quantum information research. We have developed a first principle simulation of ultra-cold ion plasma crystals in a rotating wall Penning trap. The model includes a detailed Doppler laser cooling model. This simulation has been carefully benchmarked with linear theory and demonstrates steady-state temperatures consistent with experiment. These ultra-cold two-dimensional ion crystals are being realized at the National Institute of Standards and Technology (NIST), Boulder, Colorado in a Penning trap and are being used for quantum simulation of coupled spin systems, as well as quantum sensing experiments. For the NIST Penning trap, axial motion is fairly well diagnosed which allows validation of simulation models. However, diagnostic information about the in-plane motion is not available. Stability of the crystal and control of the in-plane motion is critical for experimental advances in quantum information and this is an area where simulation can make a major contribution. The second project will explore quantum algorithms for kinetic plasma simulation. This work is complementary to the first project discussed above, in that it is a research area where fusion plasma science may benefit from future quantum computing resources. While this may seem quite futuristic and success is uncertain primarily due to nonlinearity, it is essential to begin research in this area because it requires completely rethinking algorithms. Gyrokinetic simulation (research that began over 35 years ago) of tokamak turbulence and transport can involve extreme computation with very little input and output. We have successfully formulated a quantum algorithm for the one-dimensional Vlasov-Poisson system solving linear Landau damping problem which shows a theoretical exponential speedup over the classical counterpart. Nonlinearity is a difficult challenge. We plan to explore solving the nonlinear problem using series solution involving polynomials of the initial state. We will further explore higher dimensional problems, initialization (state preparation) and measurement.