White Paper for the Decadal Survey on Biological and Physical Sciences Research in Space 2023-2032

Topical: Computation as a Vital Tool to Enable Quantitative Predictions of Many-Body Physics of Ultracold Atoms in Bose-Einstein Condensate

October 31, 2021

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SUMMARY

The Bose-Einstein condensate (BEC) and cold atom laboratory (CAL) will be built in the international space station, offering unique opportunities of experimental studies on quantum optics, atom optics, and atom interferometry taking advantage of the microgravity environment. This White Page proposes to extend the scope of the BECCAL project by recommending the investigation of many-body physics using cold atoms. The focus is on computational study, employing the most advanced and most accurate quantum mechanical methods and the latest developments in machine learning techniques, in order to provide *quantitative* predictions comparable with measured data. In this research field, an astounding gap between theory and experiment persists, and reliable computations and realistic simulations are expected to become an indispensable tool to bridge analytical models and lab measurements in near future. Specifically, the fundamental physics involved in quantum phase transitions, quantum magnetism and effects of disorder, and how to improve laser-cooling to increase the number of atoms in BEC are identified as future studies for the next decade. These studies will not only seek to solve these outstanding scientific problems, but also create and enhance collaborations between theoretical groups and experimental efforts in biological and physical sciences in space community.

I. SIGNIFICANCE

The creation of ultracold gases in Bose-Einstein condensate (BEC [1,2]) by laser cooling enables study of the fundamental physics of *many-body* interacting quantum systems [3-5], in which there exist a coherent, macroscopic matter wave. In these systems particle statistics and their interactions play a central role, leading to numerous fascinating phenomena such as the Bardeen–Cooper–Schrieffer to Bose–Einstein condensate (BCS–BEC) crossover [6] and the generation of strong effective magnetic fields [7]. Progress in this field will benefit a wide range of physics branches from condensed matter physics and statistical mechanics to high-energy physics and astrophysics. Technologically, realizing the next-generation quantum devices including quantum sensors and quantum computers depends on future breakthroughs in this field.

To reveal and understand many subtle aspects of these quantum systems, it requires a large number of cold atoms to stay in BEC with sufficient evolution time. In earth-bound conditions, gravity deforms the potential trapping cold atoms, limiting the available free-fall time, while employing a compensate field will add extra phase shifts and complicate both device techniques and data analysis. The microgravity in space eliminates the gravitational sag, allowing cold atoms remain stationary with respect to the apparatus thus greatly extending the free-fall and BEC evolution time.

The Bose-Einstein Condensate and Cold Atom Laboratory (BECCAL [8]), a collaboration between NASA and DLR (German space agency), will build BEC apparatus in the International Space Station (ISS), where the microgravity environment will extend free-fall and allow atoms to stay in BEC at macroscopic timescales (~s). In addition to the previously proposed research projects of examining the fundamental laws of physics (testing the Einstein equivalence principle, the validity of quantum mechanics on macroscopic scales, etc.), probing dark matter and dark energy, and studying quantum optics and atom optics, BECCAL will also provide unique opportunities for studying the *strongly correlated* quantum systems of ultracold atoms, currently one of the most important research frontiers in condensed matter physics and quantum physics.

This research will help to create intimate and long-term collaborations between experimental and theoretical/computational thrusts within the fundamental science community as well.

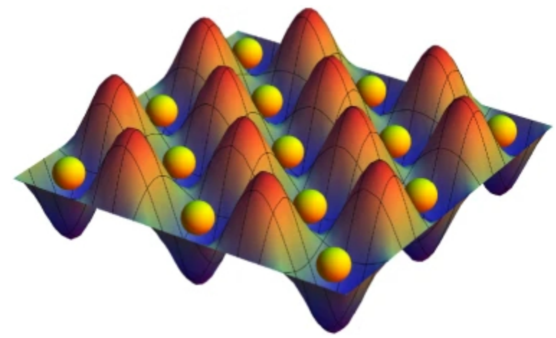

Fig. 1: Atoms located in a 2D optical lattice.

Experimentally, many-body phenomena in the strong-coupling regime can be studied by loading ultracold atoms in BEC into an optical lattice [3-5,9-11], a periodic electromagnetic potential created by the interference of laser beams as illustrated in Fig. 1 for a two-dimensional (2D) case. The perfect control and tunability of the optical lattice in potential depth and periodicity open a new approach to the investigation of numerous outstanding problems in many-body physics by continuously switching quantum phases, simplifying the electronic systems, and entering novel regimes that have not been accessed in condensed matter physics or nuclear physics.

Theoretically, in addition to analytical models which qualitatively describe the essential physics, there exist a number of highly accurate *quantitative* methods whose numerical predictions of BEC systems can be compared with measured data directly [12,13]. Nowadays computations have become indispensable for studying most of the branches of physics. However, these advanced computational methods have not been widely applied to investigate the many-body physics of ultracold atoms due to their prohibitive cost. As computer software and hardware have advanced rapidly, it is high time for such computations to be carried out routinely. In addition, machine learning (ML [14,15]) has entered the majority of scientific disciplines including quantum many-body physics in recent years, and ML will become complementary to quantum mechanical methods for numerical simulations and quantitative analysis in this field.

II. COMPUTATIONAL METHODS

Quantum Monte Carlo Methods. Quantum Monte Carlo (QMC [12, 16-19]) is ideal for the study of quantum many-body systems including ultracold atoms due to its unrivaled numerical accuracy and perfect parallelism over tens of thousands of CPUs (cores). QMC methods offer an elegant mathematical solution to the Schrödinger equation governing an interacting system. In contrast to the commonly employed effective one-particle density functional theory (DFT [20-22]), QMC accounts for the many-body interactions directly and faithfully, relying on random numbers and quantum propagators describing the evolution of a traveling particle interacting with other particles. Though DFT is extremely successful in modeling functional materials, its relatively low accuracy limits its application for cold atoms. In the next decade, methods beyond DFT are expected to enter the mainstream of quantum mechanical simulations.

For the ground-state properties of cold atoms, diffusion Monte Carlo (DMC [18]) is the recommended method. Working in imaginary time to separate the ground state wave function from those of higher-energy states, DMC is able to obtain the exact energy of a many-body system, while methods based on DFT are limited by their approximations involved and their accuracies for cold atoms are usually far from sufficient. In practice, the wave functions and energy levels computed from DFT are used to construct the initial many-body wave functions, and then DMC is performed to project out the ground state using a quantum projector.

An alternative to DMC is the path-integral Monte Carlo (PIMC [19]), which is based on the integral version of the Schrödinger equation, in comparison with DMC solving the usual differential version of the Schrödinger equation. PIMC can be carried out to obtain the exact ground-state energy at zero K. PIMC is also able to retrieve the partition function at finite temperature, then the many-body system's total and kinetical energies can be computed readily through the well-known thermodynamic relations. Furthermore, the partition function can be accurately and efficiently obtained through good approximations, making molecular dynamics (MD) simulations based on PIMC possible for studying the dynamics of ultracold atoms [23]. PIMD has been applied to compute the quantum time-correlation functions and transition state rates, which are critical to determine and understand quantum phase transitions.

Machine Learning. The past decade has seen the quick rise of machine learning in both scientific research and technological applications [14,15]. Instead of solving equations, ML seeks to recognize patterns in big data and then provides predictions. The intrinsic probability nature and extreme complexity associated with quantum many-body systems offer immense amount of data, making ML tremendously appealing in this field. In particular, the N-dimensional (N: number of particles such as electrons or photons) wave functions can be represented and parametrized using the neural-network quantum states (NNQSs) in terms of artificial neural networks [24,25]. The NNQS representations have been mainly applied in the variational data learning, i.e., in the context of variational approximations [26] to minimize the total energy of a many-body quantum system, while enforcing quantum symmetries for fermionic particles is challenging [27].

In addition to NNQS representations, one of the major applications of ML techniques in this field is to dramatically speed up QMC (and other quantum many-body) simulations [28,29]. In all these methods including DMC and PIMC, efficient sampling schemes in the N-dimensional space are often system-dependent, requiring careful tuning. The general-purpose samplers for QMC remain elusive. Unsupervised ML methods have been adopted to solve this issue for individual systems. These approaches include the self-learning MC and the generic ML models developed to accelerate sampling for specific tasks [28,29].

Another important application of ML is to identify quantum phases of many-body systems [30]. Due to the overwhelming complexity in both numerical results and experimental data, quantum phases of many-body systems are normally very hard to characterize. Supervised ML tools have been used to map out quantum phases by analyzing numerical simulations and experimental data, in combination with *a priori* theoretical knowledge and analytic modeling. The bias introduced by the chosen theories and/or models might be reduced by varying the theoretical inputs.

III. RECOMMANDED FUTURE STUDIES IN THE NEXT DECADE

Quantum Phase transitions of Ultracold Atoms in Optical Lattices. As mentioned in Part I, optical lattices offer perfect control of nearly all aspects of the underlying periodicity and the interactions between atoms located on the lattice sites. Such lattices can be 1D, 2D (See Fig. 1), or

3D, allowing explorations of a wide range of fundamental many-body phenomena such as quantum phase transitions [31-33], which could be extremely difficult to study or to realize in real materials.

Quantum phase transitions are among the central topics of many-body effects. A simple model to describe phase transitions of cold atoms in an optical lattice is the Bose-Hubbard model (BHM [34]), in which only onsite (one-particle) and nearest neighbors (two-particle) contributions are included. Though BHM is not analytically soluble even in 1D, the existence and properties of the quantum phase transitions can be qualitatively understood as functions of its parameters, e.g., the superfluid (SF) to Mott insulator (MI) transition [31-33], as the ratio of repulsion (U) to the nearest-neighbor coupling (J) increases. At $U/J \rightarrow 0$, the kinetic energy dominates and the ground state is a delocalized superfluid, while as U/J becomes large, repulsion dominates, leading to a series of Mott insulator phases with localized states. The SF-to-MI transition is associated with the loss of long-range order—the fraction of BEC density to the total density—from 1 (in SF) to 0 (in MI). These states are incompressible, and their densities remain the same when the chemical potential changes during phase transitions. A second signature of the SF-MI transition is the appearance of a finite excitation gap (Δ) in the Mott insulator, and Δ will approach U eventually.

The advantage of using cold atoms to study many-body physics is the tremendous flexibility of tuning the parameters such as U and J. One can dynamically vary the relative strength of the kinetic energy and interaction energy and study the real-time phase transitions of strongly-correlated systems in a controlled manner. Analytical models like BHM only provide general trends, while QMC and ML simulations have the potential of *quantitatively* predicting the evolution of these phases for the specific atoms in experimental or designed optical lattices, determining the values of model parameters, and characterizing and verifying the associated phase transitions.

Computation is not only the crucial bridge between theory and experiment, but also opens the door to solve many outstanding problems for future studies in the next decade.

Quantum Magnetism. Realizing and studying the configurations of cold atoms in optical lattices that can serve as tunable models for quantum magnetism [7]. Among them the fermionic repulsive Hubbard model with tunable U, J, and the BEC density fraction is of most interest to condensed matter physics, since it allows the study of the mechanism in high-temperature superconductors using cold atom in optical lattices. Though the eventual high-Tc mechanism might not be the same as found in the cold atom systems, the research will give shed new light on this long lasting problem in the heart of condensed matter physics and field theory.

There are a few possibilities pointed by analytical analysis, such as resonating valence bond states created by adiabatic spin transformation [35], and spin-liquid states on triangular [36] or Kagome-type lattices [37] which can enforce frustration in antiferromagnetic ordering. However, none of them have been successfully achieved in laboratory. Numerical simulations would be able to examine reliability of these theoretical models, find and/or design realistic magnetic systems for experimentalists to try, and provide numerical solutions to analytical models.

Effects of Disorder and Defects. Quantum impurity can affect quantum magnetism remarkably, since the diffusion of waves in a medium would be absent if certain degree of disorder is reached, the so-called Anderson localization [38]. On the other hand, strong repulsion can also cause electron delocalization (Mott insulators [39]). Therefore, in an interacting quantum system, localization of electron waves due to both disorder and repulsion can be present, which hasn't been well studied and understood from analytical models [40,41]. There are many proposals of introducing disorder or defects in optical lattices [42,43], but such investigations are particularly difficult and time-consuming, since there are countless configurations of optical lattices to impose randomness. QMC and ML simulations are expected to become the essential tool for studying disordered and/or defected optical lattices.

Improve Direct Laser Cooling to Generate More Atoms in BEC. Revealing many-body physics using cold atoms in optical lattices or building atomic interferometers using cold atoms to test fundamental physics laws require cooling more atoms to reach BEC faster. The standard laser cooling followed by evaporation creates up to 10^6 atoms in BEC, while the newly developed direct laser cooling (DLC [44,45]) overcomes the limitations of the previous technique and has the potential of reaching more than 10^8 atoms in BEC with much shorter cooling time. However, current DLC can only condensate up to 2.5×10^4 ^{87}Rb atoms below 0.6 μK [45], calling for more complex trapping strategies and better cooling processes to further ameliorate this promising technique.

Improving DLC to produce more atoms in BEC (BECCAL targets at $N > 10^8$ for testing the fundamental laws [7]) poses a significant technical challenge, since laser cooling depends sensitively on the characteristics of atomic energy levels, laser beam geometry, intensity, transverse mode, polarization, detuning energy, Doppler shift, and optical trap volume, shape, frequencies, etc. Furthermore, DLC involves multiple cooling stages; at each stage the trap potential is very different. Experimental exploration of the vast parameter space to seek new and/or better DLC designs using the trial-and-error approach is difficult and inefficient.

Therefore, reliable theoretical analysis and numerical modeling will be a very useful tool complementary to experimental efforts of improving the cooling techniques. Modeling and simulations have not been widely applied to study and optimize DLC, because DLC has only been well-developed recently, though researchers have modeled standard laser cooling (mostly optical molasses) and other relevant processes using various Hamiltonians coded for their specific cases. One approach is to solve the independent-particle Optical Bloch Equations (OBEs) to determine the dynamics of atoms subject to laser beams and trapping potentials. However, when the number of BEC atoms increases, more accurate methods such as QMC are needed to account for atomic interactions.

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