Quantum simulations with cold atoms: Fundamentals, advances, and outlook

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Abstract. Since the first proposal of quantum simulation by Richard Feynman in 1982, multiple platforms have been explored to probe the behaviour of subatomic particles, exploiting the intrinsic nature of quantum systems. As one of the most promising candidates to realise large-scale simulation, quantum simulators with ultracold gases have attracted unprecedented attention. Featuring novel detection possibilities, a high degree of controllability and the extreme physical parameter regimes that can be reached in these 'artificial solids', quantum simulation with ultracold atoms has progressively matured to the point that it can be used to study exotic quantum phenomena. This review presents the theoretical fundamentals and recent advances in related technology and offers comment on future directions.

Keywords: quantum simulation, ultracold atoms, Floquet engineering, quantum information scrambling.

1. Introduction

Ultracold atomic gases, featuring their precise controllability and tunability, have become one of the most promising candidates for quantum simulation. Major advantages of ultracold atomic clouds as quantum simulators include their inherent scalability and large coherence times. Trapped in optical lattices, which resemble the crystal structure of solids, cold atoms represent a conducive platform for the study of condensed-matter physics. In 2002, the group of Immanuel Bloch carried out a proof-of-concept experiment to illustrate superfluid Mott insulator transitions; this experiment is considered as pioneering work regarding quantum simulations with ultracold atoms [1, 2]. Studies of ultracold atoms have been extended to high-energy physics [6][7][8], statistical mechanics [16] and astrophysics [17]. This article discusses two main techniques of obtaining ultracold atoms, namely optical lattices and laser cooling. The major technological developments in this field are presented along with a section providing insights for future studies.

2. Optical lattice fundamentals

Quantum simulation with optical lattices encompasses a rich diversity of applications [pic 1]. Introduced by Soviet physicist Vladilen Letohov [8], optical lattices are periodic structures of optical potential traps for cold atoms using a standing wave generated by counterpropagating laser beams [3]. The frequency of the laser used for trapping electrically neutral atoms is selected to be well below the resonant frequency of the atoms. Two or more intersecting laser beams are combined and interfere to form a standing wave, creating crystals made of light. In addition, the arrays of peaks and valleys are used to trap atoms or molecules. The overall lattice arrangement, differing in potential well depth and periodicity, can be precisely manipulated to create desirable conditions with which to model complex quantum processes.
Optical lattices have been an indispensable tool for studies of condensed-matter physics. Spaced approximately one tenth of a nanometre apart, atoms in the lattices can represent electrons in solids. It is known that real-world solid materials are tremendously complicated structures to study. They have a convoluted band structure with a specific energy spectrum, and the Coulomb forces between individual electrons are difficult to probe. Moreover, disorder and the unavoidable vibrations of the solid lattice further compound the intricacy. Therefore, theorists have invented highly simplified models that target specific features of the system. Optical lattices have proven helpful to realise such models in experimental practice, pioneering the idea of quantum simulation [4].

3. Laser cooling

At high temperatures, particles behave in a more classical manner. Because the De Broglie wavelength can be interpreted as being inversely proportional to the square root of temperature, it is desirable to lower the temperature regime to extremity so that macroscopic quantum phenomena can be studied at scales approachable by human manipulation.

Although counterintuitive, a laser can be used to cool atomic and molecular gases from room temperature to the microkelvin regime, in which particles move with minute velocities below centimetres per second [25]. New avenues have been progressively explored with this technique, such as realising Bose–Einstein condensation exclusively through laser cooling, as well as the manifestation of continuous Bose–Einstein condensation.

The working principle of laser cooling is relatively straightforward. If a beam of photons is directed at a moving atom, the atom experiences different frequencies of the light wave (and hence momentum of photons) due to the Doppler effect. Therefore, if the initial frequency of light is tuned slightly below the targeted two-level electronic transition in the atom, the atom moving towards the laser receives the light as blue-shifted and absorbs the photon, thus slowing down. Later, the excited atom re-emits a photon in a random direction. The averaged effect of repeated absorption and emission causes the atom to be cooled.

4. Rydberg atoms

Although neutral atoms are naturally well isolated from their environments, the interactions between individual qubits tend to be weak. This phenomenon represents a major obstacle to scalable quantum computation, which is the requirement that qubits should interact intimately to produce
entangling gates and conditional logic. One approach to counteract this effect is to induce long-range interactions via the Rydberg interaction, which has been the centre of intense recent work.

Named after the Swedish spectroscopist J.R. Rydberg, Rydberg atoms possess unique and exaggerated properties. These exotic atoms have a large value of the principal quantum number \( n \), with one electron situated in a highly energised state. This single-valence electron thus experiences essentially coulombic potential and resembles a highly excited electron in hydrogen in manners. Located far from the rest of the atom, the electrostatic attraction this electron perceives is extremely weak, rendering its motion prone to perturbation or even domination by weak external electromagnetic fields. Two Rydberg-excited atoms placed at a distance apart thus perceive van der Waals dipole–dipole interactions, an advantage that can be leveraged for delivering quantum information and studying many-body spin models [26][27].

Rydberg atoms have powerful mutual interactions even when separated by large distances. The strength of the interaction can be finely tuned via the choice of excited Rydberg states and their physical separations. Rydberg–Rydberg interactions have played a pivotal role in the growing body of studies of quantum simulation, featuring the phenomenon of ‘dipole blockade’. This mechanism enables one ‘control’ atom to prevent the flow or excitation of other particles in its proximity, offering a new approach for the manipulation of quantum gates. The underlying principle is that strong Rydberg–Rydberg interactions shift the energy levels out of resonance so that under the proper conditions in an ensemble of atoms, no more than one can reach the Rydberg state.

5. **Advances in ultracold-atom platforms**

The validation of the Bose–Einstein condensate (BEC) in 1995 was a milestone for ultracold-atom technology [18]. However, this was only the beginning of a booming research field which subsequently led to a plethora of discoveries and pushed the field still further[Picture 2]. This section reviews the major advances in this technology. A more detailed discussion of ultracold gases can be found in a review article by Jook Walraven [19].

![Fig 2. Areas of studies advanced by ultracold atom platforms.](image-url)
The first atom to be captured in optical lattices was sodium, which was optically cooled to form a cloud in a magnetic trap with the help of a ‘Zeeman slower’. Later, the advent of the magneto-optical trap enabled simultaneous trapping and cooling of atoms in the same configuration [20]. Since the first BEC experiments, the exploitation of ultracold-atom platforms has been continuously broadened and has begun to overlap with condensed-matter physics. Quantum gas microscopy, for instance, is an emerging technique for precise detection that allows single-atom detection with near certainty. From 2015 onwards, several experiments have captured images of individual fermions in a lattice, the local observation of Pauli blocking, Mott insulators and so on [21].

The latest developments in the shaping of optical potentials have opened new avenues. The increasing popularity of uniform (flat-bottom) optical potential traps as opposed to conventional harmonic potentials has enabled the realisation of hitherto impossible experiments. Subsequent advances have extended into the realm of equilibrium and non-equilibrium phenomena, such as superfluidity, turbulence and the dynamics of phase transitions [22]. More specifically, box traps offer a particularly conducive environment for research regarding physical properties near critical points that are related to long-distance correlations, such as those emerging near second-order phase transitions [22].

Furthermore, the manipulation of Feshbach resonances can enable precise control over atomic interactions, leading to thermalisation in Fermi gases. Resonant scattering between ultracold alkali atoms also enables the creation of ultracold molecules from ultracold atoms via precise control. Consequently, novel occurrences such as molecular Bose–Einstein condensation and fermionic superfluidity have become realities.

6. Floquet engineering

The physical platforms that are currently exploited for quantum simulation include trapped ions, superconducting circuits, photons, and others, which can naturally engineer specific instances of many-body Hamiltonians. For example, emulation of Fermi–Hubbard [9][10], Heisenberg [11] and Ising [12] models has been demonstrated with cold atoms in optical lattices of different lattice geometries. However, in the pursuit of creating fully programmable quantum simulators, it is desirable to expand the scope of Hamiltonians that can be simulated.

One pioneering technique in this regard is Floquet engineering. Initially applied to the platform of NMR [28][29], the Floquet engineering technique imposes a periodic drive to a system to realise a wider class of periodic Hamiltonians $H(t+T) = H(t)$ with time $t$ and driving period $T$. Despite their being time-dependent, Floquet systems can be described by a time-independent effective Hamiltonian $\mathcal{H}_{\text{eff}}$ if the system is studied at multiples of the driving period. Certain properties of matter that difficult to study in a static system can be assessed by applying periodic driving. The Floquet engineering technique has led to the observation of exotic phenomena in quantum many-body systems, including symmetry breaking [13], dynamical phase transitions [14] and Floquet-topological matter [15]. The significance of Floquet engineering in studies of information scrambling is presented below.

7. Information scrambling

Equilibration, thermalisation and prethermalisation are ubiquitous phenomena that occur along with the loss of memory regarding the initial state of a system [23]. Understanding the reversibility of a quantum process is of crucial importance for quantum simulation. Ultracold-atom platforms, with their recent technological improvements, have facilitated the investigation of thermalisation of isolated quantum systems as well as the possibility of restoring initial information.

Quantum information scrambling is the spreading of local information into an entire many-body quantum system. It is currently a cutting-edge field of investigation, with promising potential in understanding the chaos in black holes as well as the fundamental nature of how causality emerges from microscopic degrees of freedom in quantum gravity. The significance of its study in relation to
quantum computation resides in the quest for reliable transmission of quantum data. Due to the experimental difficulty of direct measurement of quantum scrambling, out-of-time-ordered correlation functions (OTOCs) have emerged as an approach to characterise the degree of scrambling.

Floquet-engineering has been recently exploited to realise time-reversal Hamiltonians on NMR systems [24]; specifically, the group of Paola Cappelaro has made major contributions in this area. Time reversal allows undoing an unwanted evolution, thus restoring information that would be otherwise lost. In recent multiple quantum coherence (MQC) experiments, a pulse sequence with Floquet engineering was designed to successfully engineer a time reversal of a model Hamiltonian, revealing insights of quantum system dynamics in prethermal and thermal phases. It would be informative to perform similar experiments using cold-atom systems, drawing on experiments previously performed on NMR platforms. Based on the advances in cold-atom systems listed above, this approach appears promising.

8. Conclusion

In this review, an introduction to the field of quantum simulators with ultracold atoms has been provided, along with descriptions of technological details and working principles. The advances of this physical tool have also been discussed. In addition, the concept of information scrambling has been introduced, highlighted by the description of Floquet engineering, as well as its advised application to ultracold-atom platforms.

References

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