extended interaction *U'* need to be included. Developing understanding on smaller arrays opens an immediate route to having significant impact. At a larger scale, the behavior of the arrays cannot be calculated exactly; therefore, the experimental results can be used to benchmark quantum materials calculations against one another.

2. Cold atoms in optical lattices

Kaden Hazzard and *Bhuvanesh Sundar*

Ultracold matter has emerged as a versatile platform for engineering and exploring quantum phenomena. These gases of atoms or molecules have a density much lower than air, and temperatures at the nanokelvin-scale. Because the temperature is so low, quantum effects and interactions can play a crucial, even dominant, role despite the diluteness of the systems.

Ultracold matter was first created roughly three decades ago, utilizing dramatic advances in laser cooling and trapping.[6] In 1995, experiments produced Bose-Einstein condensates (BECs), realizing quantum degenerate ultracold matter and sufficiently large phase space densities to open a path to study interacting quantum matter.[7,8] Since then, ultracold experiments have furnished diverse types of strongly correlated matter,[9] pushed the frontiers of precision measurement and tests of fundamental physics,[10] and developed quantum technologies for quantum sensing [11] and quantum computation (note: Ref. [12] provides an illustrative example, summarizing the subfield of ultracold neutral atom quantum computation).

The payoff for achieving the extraordinary conditions of ultracold matter is the experimental capabilities that doing so enables. At such low temperatures, atoms' thermal motion is slowed to a crawl, and forces from light can affect the atoms. This allows experiments to leverage the extreme coherence of laser light to manipulate the atoms in novel ways. The unique tools of ultracold experiments rely in large part on this capability. Experiments routinely employ optical potentials to create traps with exquisitely controllable shapes, lattices with engineerable geometries, and disorder potentials with controllable strength. Interactions can be tuned from negligibly small to the largest allowed by quantum mechanics using Feshbach resonances.[13] Artificial gauge fields can be imposed.[14] The interaction range can be chosen to be negligibly short [effectively a delta-function $\propto \delta(r)$, the typical case in neutral ground state atoms] or long-ranged [for example, $\propto 1/r^3$ in dipolar molecules]. Not only does one gain these ways to control matter, but under these conditions, the Hamiltonians that quantitatively describe these systems become standard models of condensed matter physics, such as Ising models or Hubbard models. Reviews of these capabilities in the context of quantum simulation can be found in Refs. [9,15,16].

Using these tools, experimentalists have created new forms of matter. Some of these are analogs of phases of matter that occur in solid-state systems, such as superconductors across the BEC-BCS crossover (as reviewed in Refs. [17,18]), Mott insulators, and antiferromagnets.[19,20] [More recent developments than are covered in these reviews will be discussed in some detail in Sec. II Technical Appendix, Chap. 4.] Some experimental realizations are entirely new forms of matter, such as time crystals [21] and many-body localized states.[22,23] Perhaps most excitingly, whole new conceptions of quantum matter have opened up, for example phases of matter that rely on long-ranged interactions or behaviors that emerge when interacting quantum systems are coherently driven far from equilibrium.[24,25,26]

The described progress on both the experimental and the theoretical front is opening a clear path towards the long-awaited solution of the MIT puzzle in doped semiconductors. From a broader perspective, these ideas and methods should be of consequence in many other systems, for example the underdoped regime of various Mott oxides, including not only the superconducting cuprates [150] but also the equally interesting iridium oxide materials such as $(Sr_{1-x}La_x)_2IrO_4$,[151,152] which display similar physics puzzles.

3. Legacy, limitations, and prospects in view of strongly correlated Hamiltonians, including the Fermi-Hubbard model

a) Via precisely atomically-doped semiconductors

Subir Sachdev

Modern ideas on correlated quantum states should give a new perspective on older experiments on Si:P and would be valuable for understanding new structures that can be fabricated with atomic precision. Among early observations on Si:P near the metal-insulator transition was one that showed the spin susceptibility had a divergent form as $T \rightarrow 0$, and that in addition, this divergence continued smoothly across the metal-insulator transition. This is very suggestive of spin-charge separation, in the presence of inhomogeneity. In more precise terms, we can imagine that both the insulating and metallic states have topological order and require emergent gauge fields for their description. Such exotic phenomena can have observable consequences for the thermal conductivity, and lead to dramatic effects on the nature of the metal-insulator transition. Although such theories of spin-charge separated states are hard to treat analytically, considerable progress has recently been possible in the Sachdev-Ye-Kitaev (SYK) models. We will extend the SYK-type analysis to more realistic situations found in Si:P. The ability to make atomically precise structures will enable tests of the SYK analysis and extend its predictions to the vicinity of the metal-insulator transition.

b) Via optical lattices and cold atoms

Kaden Hazzard and *Bhuvanesh Sundar*

Ultracold matter already has greatly impacted our understanding of strongly correlated quantum matter, as mentioned in Sec. I (2.a.2). As a still-young and expanding field, it is too soon to write its "legacy", and as a broad field it is not possible to even survey the full landscape of results. Instead, we will focus our attention on the line of research using repulsive fermionic atoms in optical lattices to realize the repulsive Fermi-Hubbard model.[1] Even though this represents a tiny fraction of the exciting frontier of quantum simulation ultracold matter research, it provides an illustrative example of the character of much research in ultracold systems into strongly correlated matter. We provide a sketch here, with more detail in Sec. II Technical Appendix, Chap. 4.

Even in the slice of the field concentrating on fermions in optical lattices, there have been exciting advances. Landmark experiments observed the metallic phase,

[1] In solid-state physics, this is typically just referred to as the "Hubbard model," but in ultracold matter we routinely deal with bosons and fermions, so the phrase "Fermi-Hubbard model" has emerged as the standard name. We also routinely deal with both repulsive and attractive interactions, so often the name is extended further to the "repulsive Fermi-Hubbard model."

band insulator,[153] and the Mott insulator,[154,155] as well as the doping-tuned Mott-metal crossover (at temperatures above magnetic ordering). These were first observed in the 3D Fermi-Hubbard model, but have since been seen in 2D and 1D. [More discussion and citations are provided in Sec. II Technical Appendix, Chap. 4.] In the last few years, experiments have achieved lower temperatures and advanced detection techniques, and have observed short-ranged antiferromagnetic correlations in 3D and long-ranged correlations spanning the system size (~20 sites [156]) in 1D and 2D for the half-filling Fermi-Hubbard model. The current experimental temperatures, however, remain slightly above the Néel temperature T_N at which the phase transition from the normal phase to the antiferromagnetic phase occurs, by about 40% in 3D, while in 1D and 2D the Néel temperature is $T_N = 0$. Nevertheless, even these experimental regimes are at the cusp of what is tractable theoretically. Broadly speaking, with great effort theory has been able to reproduce the equilibrium experimental results, thanks to significant advances in computational methods – exact diagonalization,[157] several quantum Monte Carlo (QMC) variants, [158-160] density matrix renormalization group (DMRG),[161,162] dynamical mean field theory (DMFT),[163] and numerical linked cluster expansion (NLCE) [164] techniques have all been influential in ultracold matter – which have been driven in no small part by these experiments. However, often the systematic errors such as finite size effects of these methods are difficult to assess in this regime, and the experiments offer some of the most stringent tests of their convergence.

Prospects for the future are even more exciting. With modest decreases in temperature, the Néel phase and the phase transition properties will be accessible, and – in the system doped from half filling – even equilibrium physics lies beyond the reach of well-controlled, quantitative theory. At somewhat lower temperatures in the doped system, the putative existence of a *d*-wave superconducting phase could be studied, as could the phenomenology of any pseudogap and bad metal regimes of the model.[19,165]

However, challenges remain to reach the temperature required for these future prospects. Lower temperatures require removing entropy from the system, which is not possible in a perfectly closed system. Evaporative cooling reduces entropy and is the method used to bring atoms to ultracold temperatures, but in present conditions the cooling power provided by evaporative cooling is often balanced by intrinsic heating rates due to scattering from laser light and inelastic atomic collisions. To reach colder temperatures, the community must figure out ways to reduce the heating or find methods with sufficient cooling power to remove entropy before more is generated. Devising such methods is an outstanding goal and connects to deep physics, since understanding equilibration of these systems requires understanding transport and dynamics in strongly correlated systems.

Whatever methods are employed, current limits do not appear fundamental, and the history of cold matter suggests that major advances are still possible. As the challenges are understood and overcome, ultracold matter will impact science in even broader and deeper ways: The advances we can foresee will provide great insight into strongly correlated matter, with far-reaching consequences for quantum materials, but the unforeseen advances are sure to be the most exciting.

C. Chapter III - Cold atoms and optical lattices

Bhuvanesh Sundar and *Kaden Hazard*

Overview of ultracold matter

It is useful to view ultracold matter in the context of atomic, molecular, and optical (AMO) physics' long tradition of manipulating quantum matter with increasing levels of control, illustrated in Figure 14. In the 1800s and early 1900s, experiments were measuring the quantized electronic spectra of gases of atoms, as shown in Figure 14(a). These measurements ushered in quantum mechanics, as just one of their profound impacts. The ability to precisely measure spectra naturally lead to the ability to control atoms' electronic states, pumping them into desired excited levels. The invention of the laser in the late 1950s and 1960s revolutionized the ability of physicists to control these excitations, allowing desired electronic states to be populated, including high-fidelity quantum mechanical superpositions of different energy levels [Figure 14(b)].

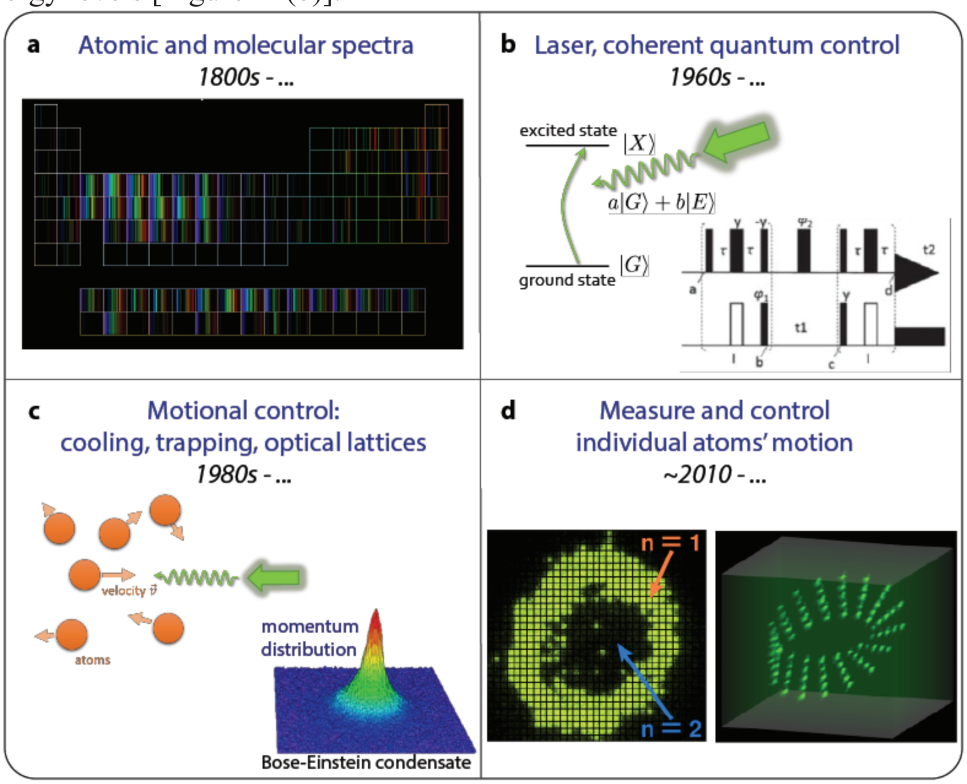

Figure 14. Increasing control of quantum matter in AMO physics through history. (a) Emission spectra of the elements. (From Ref. [107].) (b) Control of coherent quantum superpositions of electronic levels. (Adapted from Ref. [108]) (c) Controlling motion of many atoms: laser and evaporative cooling, optical trapping, and new states of matter such as Bose-Einstein condensates. (Momentum distribution adapted from Ref. [109]) (d) Measuring and controlling many-body motional states atom-by-atom: quantum gas microscope (left, adapted from Ref. [110]) and programmable optical tweezer arrays (right, adapted from Ref. [111]).

Lasers can control not only the internal state of the atoms, but also their motion in space, as demonstrated in the 1980s [112].[1] This new layer of control, specifically the techniques to cool and trap atoms that are now universally used in ultracold experiments (Figure 14c), ushered in a new era. A landmark application of these tools was to combine them with evaporative cooling[2] to create a new state of matter, dilute Bose-Einstein condensates (BECs), in 1995.[115] In this state, despite being dilute – a million times less dense than air – the indistinguishable atoms overlap and quantum statistics play a major role. Bosonic statistics compel the particles to coalesce into identical quantum states, roughly the lowest single-particle energy state. This was the first example of many-body quantum degenerate matter in ultracold systems.

A great virtue of studying matter at these low temperatures and densities is that the atoms move so slowly that they are susceptible to the tiny forces generated by light and magnetic fields. Such forces are used to generate traps for the atoms as well as the lattices that are crucial to realize the Fermi-Hubbard model. These forces are now used to image and control many-body quantum systems atom-by-atom.[116,117] The exquisite level of control of these systems makes them natural candidates for *quantum simulators* of strongly correlated matter.

Henceforth, we will concentrate on quantum simulations of the Fermi-Hubbard model with ultracold fermions in optical lattices. Our reasons for focusing on this case are not that it is the only example of a model simulated in ultracold matter, or even the most important or exciting. In actuality, numerous states of strongly interacting matter and phenomena have been explored in ultracold matter. Several are mentioned in Sec. I, and even these encompass only a tiny fraction of those studied in experiments.

Rather, there are two important reasons we focus on the Fermi-Hubbard model. First, it is the most relevant point of comparison for the 2D Quantum Metamaterials Workshop and has some of the most familiar connections to strongly correlated condensed matter. Second, exploring this model and its ultracold realizations will illuminate many general themes of ultracold matter – its successes, limitations, and potential.

A comprehensive and up to date review focused on quantum simulation of the Fermi-Hubbard model in ultracold matter can be found in Ref. [118].

The rest of this appendix material is organized as follows. The first section provides background on what ultracold matter is, typical length and energy scales, and important measurement techniques. The next section discusses how the Fermi-Hubbard model arises in these systems. Next, the section “Achievements of cold atom Fermi-Hubbard experiments” outlines the main achievements of ultracold realizations of the Fermi-Hubbard model in the context of quantum simulation. The final section discusses next steps, challenges, and prospects for the future.

A primer on ultracold matter

Ultracold matter refers to dilute gases of atoms or molecules trapped in high vacuum and at very cold temperatures. Broadly, the goal of most experiments on ultracold matter is to simulate phenomena with a high degree of control. To avoid

[1] Cooling and trapping of neutral atoms were demonstrated in the 1980s. In trapped ions, laser cooling had been proposed and implemented in 1978.[113,114]

[2] Fundamentally, this is the same process that cools a cup of hot coffee to room temperature. Hot atoms evaporate out of the trap, which has a finite depth. In practice, experiments tune the depth of the trap as a function of time to optimize this evaporation efficiency.

unwanted interactions of atoms/molecules with the environment and with each other (such as chemical reactions), experimentalists work with a dilute gas that is isolated from the environment. A typical experiment has about 10^5 particles in a small cloud roughly100 μm in size in the middle of a vacuum chamber, resulting in a density of ~10^{12} cm^{-3}. Because the density is so low (for comparison, 7 orders of magnitude lower than air), the temperature of the gas should also be low to observe quantum effects. The temperature for this is such that the inter-particle spacing is around or smaller than the thermal de Broglie wavelength of the atom/molecule, $n^{-1/3} \sim \lambda_{th}$, yielding a nano-Kelvin scale temperature. Cooling gases to such a low temperature is the price that experimentalists pay to achieve precise control and eliminate unwanted interactions.

The popular workhorses for ultracold matter are the alkali atoms - lithium, sodium, potassium, rubidium, and cesium, owing to their simple electronic structure; all of them have one valence electron. Many of the alkali have multiple isotopes some of which are bosonic and some fermionic. Working with different atomic species requires different experimental conditions. However, researchers have cooled all these atomic species to nano-Kelvin scale temperatures (see [119-122] for reviews). New atomic species are being added to the list at a rapid pace, which now includes alkaline-earth-like atoms such as strontium and ytterbium, [123,124] as well as open-shell lanthanides such as erbium and dysprosium.[125,126] The development of techniques to create degenerate quantum gases of all these atomic species is driven by each one's unique advantages - some have simple electronic structures, while some others may have highly metastable excited states, and yet others may have strong magnetic dipole interactions. Experimentalists often work with atoms in the lowest hyperfine state, although higher hyperfine states or even excited electronic states may be used as well. The Zeeman states in the lowest hyperfine manifold act as a pseudospin, analogous to the spin of an electron in condensed matter physics. Other forms of ultracold matter of recent interest are alkali atoms in highly excited Rydberg states (n > 50), and ground-state bialkali molecules such as KRb, NaRb, NaK, and RbCs.[127-131]

In a typical experiment, a gas of atoms is emitted from a source such as a chunk of alkali metal in an oven, cooled in several stages such as laser cooling and evaporative cooling, and then trapped in vacuum by magnetic fields and/or light. An important question in all experiments on ultracold matter is the time scale in the experiment. In principle, a dilute gas of ultracold atoms is never in equilibrium, as the ground state is always a chunk of metal. Nevertheless, the gas is metastable over the duration of the experiment, which may be a few seconds, and therefore can attain thermodynamic equilibrium within the metastable phase space.

After cooling and trapping a gas, researchers couple the particles to external fields that are appropriately tailored to study the desired physics. The most common ways to interact with atoms/molecules is electromagnetic radiation (UV, visible, microwave, and rf) and static magnetic fields (up to several hundred Gauss). For example, researchers may load the particles into a lattice created by a standing wave of light to realize Hubbard or other lattice models (see Sec. B for details). Researchers may also perform several experiments that do not involve a lattice, but instead require a homogeneous ultracold gas. Magnetic fields may be used in an experiment to trap atoms, as well as tune the interaction strength between atoms via a Feshbach resonance.[132]

An experiment typically concludes by taking an image of the gas, which measures the density of the gas at different points in space. Here, researchers use probing techniques that are unique to ultracold atoms. In one technique called "time-of-fight measurement", researchers turn off the trap and let the gas expand for a few hundred ms, and then capture an image using a camera. The time-of-flight measurement yields information about occupation in different momentum states; and, for example, straightforwardly discerns condensate and insulating phases. Another measurement technique that was developed recently for experiments on lattices is quantum gas microscopy,[116] which measures the number of atoms on each lattice site in-situ. Developments in quantum gas microscopy have enabled researchers to study various phenomena, such as phase diagram of the Bose-Hubbard model,[133] localization in the Aubrey-Andre model,[134-136] and a direct measurement of the entanglement entropy,[137] as just a few examples, as well as the physics of the Fermi-Hubbard model, as we'll see in more detail below.

How the Fermi-Hubbard model is realized in ultracold matter

In this section, we describe how the Fermi-Hubbard model arises as a quantitative description of ultracold fermions in optical lattices,[138] and how experiments achieve their high degree of control of the lattice and system parameters. Experiments can make artificial crystals – specifically, periodic potentials for the atoms – known as optical lattices by interfering laser beams,[115] which control the tunneling and on-site interaction between atoms by tuning the laser intensity. Additionally, the interactions can be controlled by tuning a magnetic field. This allows experimentalists to accurately simulate the Hubbard model over a wide range of tunneling-to-interaction ratios.

In contrast to naturally occurring solid-state systems, the Hubbard model is not simply a toy model that captures some essential physics. Rather, it is a quantitatively accurate, rigorously derivable model for atoms in optical lattices in the ultracold regime. Here, we explain in detail the ingredients to simulate the Hubbard model for cold atoms, and from these ingredients derive the Hubbard model as a description of the system.

To create a potential for atoms using light, experimentalists use the AC Stark shift [115] that results from coupling to light that is far detuned from an atomic transition. To understand this, consider an electromagnetic field of frequency illuminating a two-level atom with an energy difference $\hbar\omega_0$ between the two levels, as shown in Figure 15(a). The detuning of the laser from the excited state is $\delta=\omega_0-\omega$. The light does not couple to any other atomic levels that are nearby in energy, and therefore to a good approximation, the atom can be assumed to be a two-level system. The atom may also carry a pseudospin index, which we will introduce later. The Hamiltonian for the system is

$$\hat{H} = \hbar\omega_0 \, |e\rangle\langle e| \; + \; \hat{H}_{atom-light},$$

where $\hat{H}_{atom-light}$ describes the coupling between the atom and light, given by

$$\hat{H}_{atom-light} \; = \; \hat{\vec{d}} \cdot \vec{E} \, cos\,(\omega t) \; = \; d_{eg} E \, cos\,(\omega t) \, (\, |g\rangle\langle e| + |e\rangle\langle g|),$$

with $\hat{\vec{d}}$ the dipole operator and $\vec{E}$ the electric field amplitude.

In the frame rotating at a frequency ω, the rotating wave approximation is highly accurate and yields the effective Hamiltonian

$$\hat{H} = \Omega(|e\rangle\langle g| + |g\rangle\langle e|) + \hbar\,\delta|e\rangle\langle e|,$$

where $\Omega = d_{eg}E/2\hbar$. Finally, in the limit where the detuning $\delta \gg \Omega$, we eliminate the excited state $|e\rangle$ using second-order perturbation theory, and obtain the low-energy Hamiltonian

$$\hat{H}_{eff} = -\frac{\hbar\,\Omega^2}{\delta}\;|g\rangle\langle g|.$$

This is called the AC Stark shift.[115] It is a potential energy for an atom that is proportional to the intensity of the laser, and inversely proportional to the detuning of the laser from atomic transition from $|g\rangle$ to $|e\rangle$.

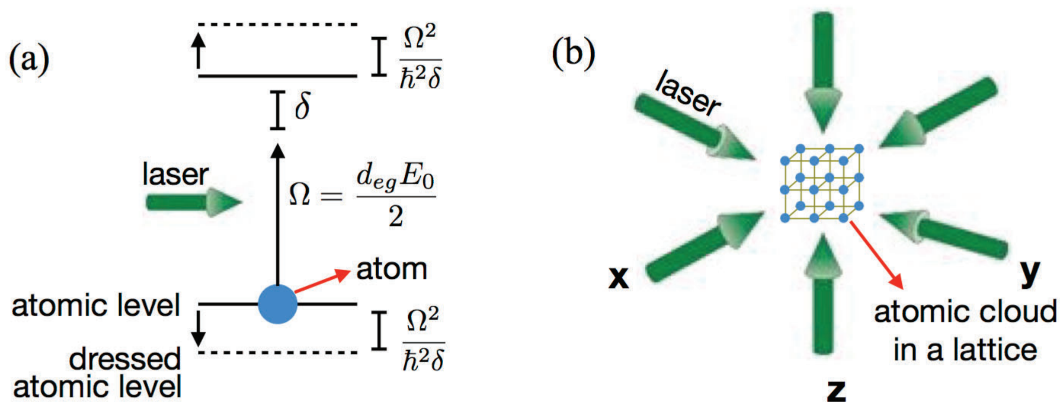

Figure 15. (a) Illustration of the AC Stark shift for a two-level atom illuminated by far-detuned light. The energy of the dressed atomic levels is shifted from the bare atomic levels by an amount proportional to the intensity of the light. (b) Schematic of a laser configuration used to create a cubic optical lattice. Other lattices may be created by adjusting the laser configuration.

Experimentalists create an optical lattice for the atoms by interfering two counter-propagating laser beams.[115] The intensity of the interference pattern modulates periodically in space, resulting in a periodic potential for the atoms. The effective Hamiltonian for the atoms (not yet including the interaction) is

$$\hat{H} = \sum_\sigma \int d^3\vec{r}\,\hat{\psi}_\sigma^{\dagger}(\vec{r})\,\left(-\frac{\hbar^2\nabla^2}{2m} + V(\vec{r})\right)\hat{\psi}_\sigma(\vec{r}),$$

where $V(\vec{r}) = V_0\cos^2(\vec{k}\cdot\vec{r})$ is the periodic potential created by the interfered laser beams, V_0 is the lattice depth proportional to the intensity of the lasers, $\vec{k}$ is the wave vector of the periodic modulation, and $\hat{\psi}_\sigma(\vec{r})$ is the annihilation operator for an atom with spin σ at $\vec{r}$. A schematic of the setup is shown in Figure 15(b).

The periodic potential created in this manner is free of defects or dislocations. Different lattices can be created by tuning the laser configurations, and their directions and polarizations; *e.g.* researchers can create a 1D lattice, 2D lattices such as square, triangular,[139,140] honeycomb,[140,141] Kagome,[142] 3D lattices such as a cubic lattice and various kinds of superlattices.[143-146]

The Hamiltonian that describes atomic motion in a deep optical lattice (treating only the non-interacting part) is the tight-binding Hamiltonian. To see this, write the field operator as $\hat{\psi}_\sigma(\vec{r}) = \sum_i\ \phi_i(\vec{r})\hat{a}_{i\sigma}$, where $\phi_i(\vec{r})$is the Wannier function for the lowest Bloch band localized at the lattice site labeled i, and $\hat{a}_{i\sigma}$ annihilates an atom of spin σ from the lowest Bloch band at the site i. Substituting the field operator in the Hamiltonian, we obtain [138]

$$\hat{H}_{TBM} = -t \sum_{\sigma,<ij>} \hat{a}_{i\sigma}^{\dagger} \hat{a}_{j\sigma}, \text{ where}$$

$$t = -\int d^3\vec{r}\, \phi_i^*(\vec{r}) \left(-\frac{\hbar^2\nabla^2}{2m} + V(\vec{r})\right) \phi_j(\vec{r}).$$

Here, t is the tunneling amplitude, and the sum in $\hat{H}$ runs over neighboring sites i and j. The tunneling amplitude can be directly controlled by the laser intensity and/or detuning. For example, increasing the lattice depth localizes the Wannier functions more, thereby decreasing t. In principle, longer-range tunneling and operators involving higher bands are present. However, the next-nearest-neighbor tunneling amplitude is typically small due to negligible overlap between those Wannier functions. And because the temperature (and interactions treated below) are much smaller than the band spacing, occupation of higher bands is negligible.

In addition to the tight-binding Hamiltonian above, the atoms have van der Waals interactions. The range of this van der Waals interaction, ~ few nm, is much smaller than typical inter-atomic spacing, ~μm. In this limit, the van der Waals interaction is well-approximated by a delta function pseudopotential, $V_{int}(\vec{r}) = \frac{4\pi\hbar^2 a_s}{m}\delta(\vec{r})$, characterized by a single parameter - the scattering length a_s. Similar to the non-interacting Hamiltonian, we can project the interactions on the lowest-band of the lattice, and only retain the on-site terms. For a pseudospin-½, this leads to an effective on-site interaction between the atoms,[138]

$$\hat{H}_{int} = U \sum_i n_{i,\uparrow} n_{i,\downarrow},$$

where $n_{i,\sigma} = a_{i,\sigma}^{\dagger} a_{i,\sigma}$ and

$$U = \frac{4\pi\hbar^2 a_s}{m} \int d^3\vec{r}\, |\phi_i(\vec{r})|^4 .$$

The interaction strength U can be controlled by tuning the lattice depth. For example, increasing the lattice depth localizes the Wannier functions more and increases the overlap of the Wannier function on a site with itself, thereby increasing U. Experimentalists can controllably tune U/t over several orders of magnitude by adjusting the lattice depth. Another technique to tune U is to adjust the scattering length a_s, achieved by tuning a magnetic field near a Feshbach resonance, which shifts the energy of a two-atom bound state relative to the energy for unbound atoms.

Together with $\hat{H}_{TBM}$ and $\hat{H}_{int}$, the total Hamiltonian for the atoms in an optical lattice is the Hubbard model,

$$\hat{H}_{Hubbard} = \hat{H}_{TBM} + \hat{H}_{int}.$$

Extensions to the Hubbard model

In addition to producing the Hubbard model given above, experiments on ultracold atoms also enjoy the luxury of adding more ingredients to the system in a controllable manner. Some pursuits that have become popular recently have been the addition of strong artificial magnetic fields, disorder with controllable strength, higher Bloch bands in the lattice, SU(N)-symmetric interactions, and long-range interactions, to name a few. Here, we elaborate on some of the ideas to add these ingredients.

Neutral atoms do not feel a Lorentz force from a real magnetic field, an essential ingredient to simulate phenomena such as the Harper-Hofstadter model,[147] and integer and fractional quantum Hall effects.[148] Therefore, researchers devise schemes to produce strong artificial magnetic fluxes for cold atoms by coupling them to light that has been tailored accurately. A large magnetic flux per plaquette is achieved [149-151] by inducing complex hopping amplitudes between lattice sites, which introduces a Peierls phase for the atoms. To accomplish this, researchers turn on a lattice tilt along one direction, say the $\hat{x}$ direction, so that hopping is suppressed along $\hat{x}$. Then, researchers reintroduce hopping along $\hat{x}$ by shining two Raman lasers that drive photon-assisted tunneling; an atom absorbs and emits a photon to tunnel from one site to the next. In the process of absorption and emission, the atom also picks up a complex phase due to the spatial phase of the electromagnetic field. The magnetic flux per unit cell induced in this manner can reach values as large as the flux quantum $h/2e$, which would require applying more than 1000 Tesla in a solid-state system.

Researchers can introduce quasi-randomness in optical lattices by superposing two optical lattices with incommensurate periodicities.[134,136] This technique has been used to study many-body localization of fermions in 1D systems, opening prospects to study many-body localization in higher dimensions. In fact, researchers have already been exploring this phenomenon in two dimensions for bosons.[135]

Atoms can be controllably excited or coupled to the higher Bloch bands of an optical lattice by various means, such as shaking the lattice,[152,153] resonant transfer by introducing an energy bias between sites,[154] and two-photon Raman transitions.[155] These schemes allow researchers to study unconventional forms of superfluidity.

It is possible to go beyond the Hubbard model interactions by performing experiments with different kinds of ultracold matter. For example, in alkaline earth atoms, which have a large nuclear spin, the on-site interaction between atoms have full SU(*N*) symmetry,[123] where *N* can be as large as 10 for some species such as ^{87}Sr. Using these species, it is possible to simulate the SU(*N*) Heisenberg model, and other SU(*N*)-symmetric Hamiltonians which have exotic ground states such as spin liquids and valence bond solids.[123] Other kinds of many-body ultracold matter in optical lattices, such as ultracold molecules,[127-131] Rydberg atoms,[156-161] and dipolar atoms such as chromium or some lanthanides,[162-164] have long-range dipole interactions extending beyond the on-site Hubbard-type interactions. These long-range dipole interactions potentially have lots of applications as well, producing new phases such as density wave orders and *p*-wave superfluids, to multi-qubit operations in quantum computation.

Achievements of cold atom Fermi-Hubbard experiments

To go from experimentally achieving a BEC to realizing the Fermi-Hubbard model, experimentalists needed two crucial ingredients: an optical lattice using the techniques discussed in the previous section and ultracold fermions. To explore the exciting physics of a lattice system near the Mott insulator phase, it is crucial to work in a regime that is cold compared to the band spacing and at a filling of roughly one atom per site. Each of these ingredients represent substantial lines of research, with broad impacts in their own right.

Researchers first created bosons at temperatures and densities where the Mott insulator physics manifests in 2002.[165] By varying the lattice depth to change the ratio of interaction to tunneling, they observed the system transition from a bosonic Mott insulator to a superfluid. The Mott insulator occurs when interactions are strong relative to the tunneling and the system is near an integer number of particles per site. Then the energy cost for an atom to tunnel, causing a deviation of the local density from its integer value, will suppress the motion of the atoms, leading to an insulating state. These conditions paved the way for experiments probing numerous properties (momentum distributions, real space correlations with single site resolution, spectra, transport properties, …) across the quantum phase transition in various conditions. The variety of situations has included 1D, 2D, and 3D lattices, as well as controllable disorder that can be turned on or off at will. These experiments thus proved to be, as suggested in Ref. [166], powerful quantum simulators of the Bose-Hubbard model, a "toy" model that had been introduced for granular superconductors more than a decade prior.[167]

Contemporaneously, experimentalists produced the first quantum degenerate gases of fermionic atoms in 1999. These atoms were in a mixture of two hyperfine states, thus forming effective spin-½ systems. It was necessary to use multiple spin states to enable the collision processes that are essential for equilibration during the cooling process, since identical fermions lack *s*-wave collisions and thus are effectively non-interacting at the low temperatures being studied. Fortuitously, spin-½ fermions are also the essential building blocks of many interesting strongly-correlated phenomena, such as superconductivity and the Fermi-Hubbard model.

Besides the Fermi-Hubbard experiments that we will focus on, these degenerate Fermi gases led to exciting new fields in their own right. For example, attractive Fermi gases with interactions controlled by a Feshbach resonance were used to create analogs of superconductors in 2004-2005, as reviewed in Ref. [168]. They subsequently have been used to study strongly correlated superconductivity, for example the BEC-BCS crossover and exotic superconductors, such as the Fulde-Ferrell-Larkin-Ovchinokov (FFLO) state.

Realizing the Fermi-Hubbard model by combining ultracold fermions with optical lattices was a natural goal for the community, with potential for huge scientific payoffs. This was driven in large part by the scientific interest in the Fermi-Hubbard model, which stemmed from two sources. First is the Fermi-Hubbard model's connections to high-temperature superconductivity, with it forming a minimal model often believed to capture essential physics of the cuprate superconductors. The second is the Fermi-Hubbard model's status as a standard model for strongly correlated physics that lies at least partially out of the reach of well-controlled numerical methods.

The first efforts loaded fermionic atoms into optical lattices and observed the interplay of quantum statistics with the band structure. Specifically, researchers [169] observed that spinless fermions with one particle per site form a band insulator, and (at lower densities) a metal, as shown in Figure 16(a). These experiments were an exciting new direction for ultracold matter, but much of the essential physics did not involve interactions, and they were far from the Mott regime.

The first experiments in ultracold matter to explore Mott physics in the Fermi-Hubbard model were in 2008, in the groups of Tilman Esslinger [171] and Immanuel Bloch.[172] These experiments revealed the finite-temperature crossover from a metal to a Mott insulator. Two of the primary observations were a suppression of double occupancies and a significant dip in the compressibility when the system was near half-filling (one atom per site) and U/t was large. More recent measurements of this are shown in Figure 16(b). Similar to the Bose-Hubbard model, in this limit, there is a gap to density excitations from the state with one atom per site, and this gap was also observed in spectroscopic measurements by modulating the lattice depth. An important feature in all of these experiments is the presence of the trap, which means the density varies throughout the system, starting largest in the center and dropping as one progresses to the edges. For a slowly varying trap, one can think of the system as being composed of a homogeneous subsystem with a large chemical potential in the center decreasing and becoming negative as one works out to the edge. The density

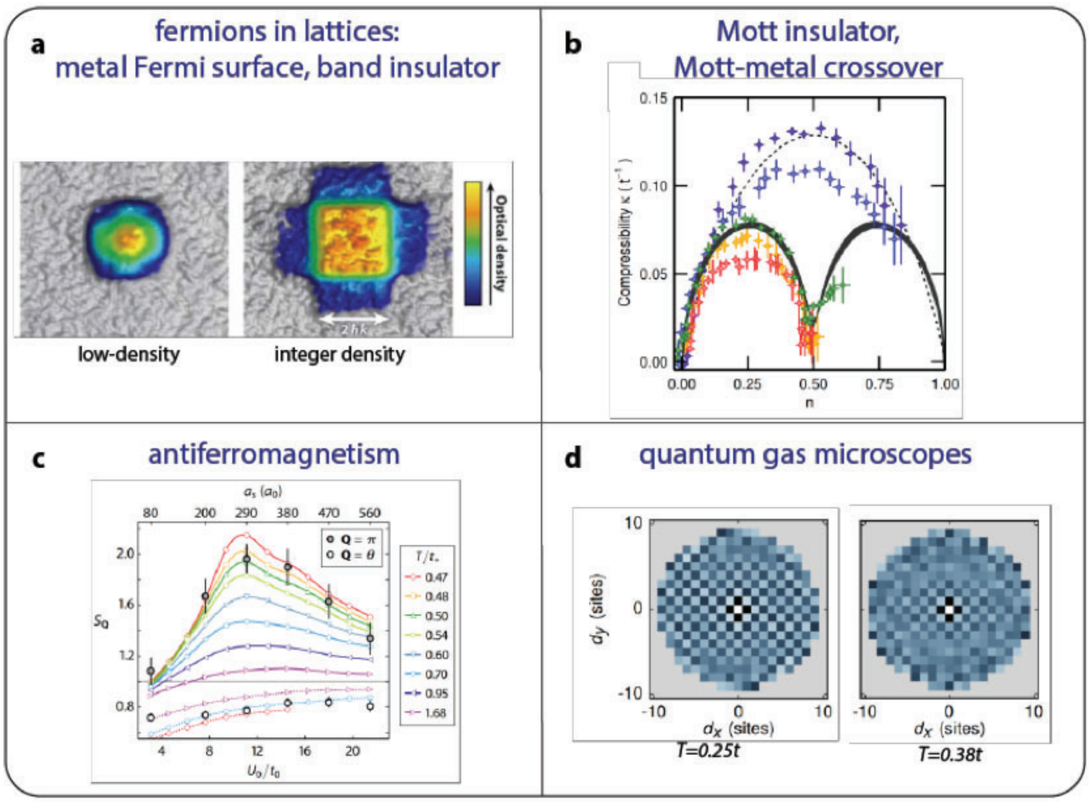

Figure 16 Milestones in quantum simulations of the Fermi-Hubbard model with ultracold matter. (a) Observation of Fermi surfaces in lattices: momentum distributions measured by time-of-flight for two densities. (Adapted from Ref. [170].) (b) Precision measurements of Mott-metal equation of state for a number of interaction strengths from U = 0 to U = 20 t (different colored points) compared with non-interacting theory (dashed line) and U = 8 t theory from the dynamical cluster approximation (grey band), which agrees with the U = 8 t experimental data (green points). (Adapted from Ref. [176]) (c) Observation of strong antiferromagnetic correlations in 3D, above T_N. This shows the structure factor for the antiferromagnetic wavevector, $S(\pi)$, and zero wavevector, $S(0)$, as a function of U/t compared with theory (solid lines connecting circles) at various temperatures. (Adapted from Ref. [187]) (d) Observations of real space spin-correlations $\langle S_i^z S_j^z \rangle - \langle S_i^z \rangle \langle S_j^z \rangle$ summed over all i and j, in a quantum gas microscope. (Adapted from Ref. [191])

will therefore decrease as one approaches the trap edge, but it will be nearly constant in the incompressible region of the trap.

Experiments on the Fermi-Hubbard model's Mott-metal crossover have proliferated. Experimentalists have measured accurately how the equation of state – *i.e.* the density as a function of chemical potential $n(\mu)$ – by measuring how the density varies in the trap, as well as double-occupancies and the nearest neighbor correlations.[171-174] In addition to these 3D cubic lattice experiments, similar experiments have been performed in 2D square lattices,[175-178] 2D honeycomb lattices,[179] and near 1D, as well as in anisotropic lattices interpolating between 1D and 3D.[180]

In addition to exploring this variety of lattice geometries, experiments have measured properties of generalizations of or other regimes of Fermi-Hubbard models. They have explored the attractive ($U < 0$) Fermi-Hubbard model,[181] and the spin-imbalanced Fermi-Hubbard model.[182] Experiments with Yb atoms have created and studied Mott insulators in Fermi-Hubbard models with SU(*N*) symmetric interactions for *N* as large as *N*=6.[183,184] Experimentalists have also developed novel environments and probes, for example by coupling a 1D mesoscopic Fermi-Hubbard wire to fermionic reservoirs, making analogs of transport experiments possible.[185]

Although many experiments have studied the Mott insulator-metal crossover, the most interesting physics of the Fermi-Hubbard model also involves two other essential types of phenomena, with their own characteristic energy scales. (1) If the system is not exactly at half-filling, holes (sites without atoms) and doublons (sites with an extra atom) will tunnel, with characteristic energy t. (2) Spin correlations develop between particles in (or near) the Mott insulator. Specifically, being in a Mott insulator does not determine the behavior of the spin degree of freedom: as long as the system is dominated by configurations where each site harbors a single fermion, the spin degree of freedom of that fermion is free. However, there are effective spin-spin interactions. In the $U \gg t$ limit, these emerge from superexchange with a characteristic scale $\frac{t^2}{U}$. In the $U \ll t$ limit, these have a characteristic scale $U\, e^{-a\, U/t}$, for some constant a. In both cases, the effective interactions drive the system towards an antiferromagnetic state. In 3D systems, there is a finite temperature phase transition to an antiferromagnetically ordered Néel state at temperature T_N, while in lower dimensions there is finite (possibly very long) range order at finite temperature. In either case, the energy scales associated with these phenomena are often substantially less than *U*, and so, while achieving $k_B T \ll U$ suffices to experimentally explore the Mott-metal crossover, even lower temperatures are needed to explore physics associated with the spin correlations or the physics, such as potential superconductivity, arising when the density deviates from half filling.

In the last few years, experiments have begun to explore antiferromagnetic spin correlations associated with these smaller energy scales. This has been facilitated by a combination of colder temperatures and more refined experimental probes. [180,186-194] Two particularly important tools in this context are Bragg scattering and quantum gas microscopes.[116] The latter refers to experiments with the ability to measure every site of a 2D lattice, *i.e.* the location of each atom in the lattice. This allows experiments to extract not only average densities with extreme spatial resolution, but also two-site (and higher) correlations of density and spin. Of particular importance is the observation of significant antiferromagnetic correlations, extending out to a range of several sites.

In particular, in 3D cubic lattices, experiments reached temperatures of roughly $T \sim 1.4\, T_N$ ($T \sim 0.5t$ and $U \sim 10t$) and measured the Bragg scattering signal at a wavevector commensurate with the expected antiferromagnetic ordering. They observe a substantial Bragg signal, which corresponds to a correlation length of roughly one lattice spacing [see Figure 16(c)]. Put another way, a spin on one site is strongly correlated with its six neighbors and has non-negligible correlations with a larger shell.

In 2D square lattices, the strongest correlations and lowest temperatures have been reached in experiments that use quantum gas microscopes. Although true long-range order is forbidden at non-zero temperature for the SU(2) symmetry-breaking antiferromagnet in dimension two or lower, so $T_N = 0$, the longest-range antiferromagnetic correlations have in fact been observed in 2D. The longest ranged correlations have been reported in Ref. [191], who achieved temperature $T \leq 0.25\, t$. They observe non-negligible correlations across the whole system, roughly a circle containing 80 sites (*i.e.* a diameter of about 10 sites), with an exponential correlation length of about $\xi \sim\ 8$ sites [Figure 16(d)].

It is worth noting that the majority of these experiments in both 2D and 3D are at or beyond the frontier of what can be quantitatively calculated numerically in a well-controlled fashion. For $T \sim\ t$ or higher, several numerical techniques can satisfactorily reproduce the equilibrium observables and equal-time correlations. Frequently used techniques include full exact diagonalization (ED),[195] determinantal quantum Monte Carlo (DQMC),[196] single-site dynamical mean-field theory (DMFT),[197] diagrammatic Monte Carlo,[198] and the numerical linked-cluster expansion (NLCE).[199] DQMC and NLCE have become the methods of choice, with DQMC often preferred for smaller U/t and NLCE for larger U/t. However, at the frontier of temperatures $0.25t < T < t$, these numerical methods cease to be well-controlled, in the sense that there are numerical inaccuracies (for example, finite-size effects) whose size may be significant, which are difficult to systematically evaluate under these conditions.

So far by judicious choice of algorithm and the employment of large-scale computer resources, numerical calculations have been able to reproduce experimental observations. However, due to the difficulty of directly assessing the numerical convergence explained above, the comparison with experiment provides arguably the best evidence that these methods are accurate in the regime of comparison. In this way, we are at the exciting time where experiments done in the present conditions give us information beyond the ability to be confidently extracted from numeric procedures. Note the discussion by Richard Scalettar and Ehsan Khatami in Section II, Chapter 2.

Prospects, challenges, and future directions

Future directions. While ultracold experiments have already enhanced our understanding of the Fermi-Hubbard model, there are several clear next steps for these experiments with even greater impact. Achieving temperatures sufficient to reach the antiferromagnetically ordered state in 3D, *i.e.* $T < T_N$, is a major goal. Once achieved, this will allow experimentalists to apply the powerful tools of ultracold matter to studying a super-exchange-driven magnetically ordered phase, including the critical phenomena associated with the magnetic phase transition. Moreover, once such temperatures are within reach, there are numerous parameters to vary to explore the different physics. For example, experiments could implement different lattice geometries to study frustrated magnetism, apply disorder and study its effects, and engineer topological band structures to investigate the interplay of topology and interactions. Diverse phenomena will become immediately accessible.

A long-time motivational goal for the field, and a logical next step after antiferromagnetic order is achieved, is to realize the *d*-wave superconducting phase that is widely predicted to occur in this model, or to rule out its existence. To do this, experiments must study the same system away from half-filling and at even lower temperatures than the Néel temperature, perhaps by a factor of 2 or 3. If such temperature can be reached, and suitable measurement tools applied, ultracold experiments will be able to directly probe a phase of this model that has been intensely debated for more than 30 years.

Perhaps the most interesting physics in the Fermi-Hubbard model may not even require achieving such low temperatures. Two phenomena of particular interest are possible pseudogap and the bad metal regimes of the Hubbard model. Studying these phenomena in ultracold matter may be possible in the near term, and in doing so would lead to profound new insights about quantum materials.

The first of these phenomena, the pseudogap, is displayed in many materials, which have a strongly suppressed density of states resembling an energy gap. There are many mechanisms that can give rise to a pseudogap, some mundane and some exotic.[200] The second of these phenomena, bad metals, occur in numerous materials, including high-temperature superconductors.[201] The question of what gives rise to the pseudogap and bad metal behavior in the cuprates (and other materials), specifically whether these behaviors are captured by the Hubbard model, is one that can potentially be addressed in ultracold experiments.

Challenges. Many of the phenomena described above require lower temperatures than have been demonstrated to date; but, encouragingly, the majority may occur within a factor of two or so of the current state of the art. The key challenge to reaching lower temperature is to remove entropy from the system faster than it is added by inevitable heating processes.

In present experiments, entropy is removed by evaporative cooling, which reduces the entropy by transporting high energy particles out of the trap. However, as experiments explore physics at lower energy and temperature scales, the characteristic timescales get longer, and entropy transport becomes very slow. This is compounded by the fact that it needs to be transported across the whole system, for example from the center to the edge. Given that the system may even be in an insulator, transport is essentially frozen over the lifetime of the experiment, as elegantly demonstrated in the Bose-Hubbard model.[202] Meanwhile, heating occurs due to inelastic collisions and light-scattering from lattice and trap lasers.[203] The key for progress is then finding regimes to minimize heating processes, and devising more efficient schemes to remove entropy than simple evaporative cooling. Speeding up transport, and in particular avoiding the necessity to redistribute entropy across long distances via slow transport processes, seems crucial.

Although there are challenges to overcome, they are not fundamental. With reasonable advances, we expect ultracold matter to reach into unprecedented regimes of the Fermi-Hubbard model and its relatives. In the process, we will learn even more about strongly correlated fermions. This will certainly include phenomena that are already of great interest – antiferromagnetism, *d*-wave superconductivity, pseudogap, and bad metal behavior. Moreover, there are dozens of models beyond the Fermi-Hubbard model and other phenomena being explored, each exciting in its own right. The biggest advances will surely be surprises that we have yet to anticipate.

D. Chapter IV - Real time control of Hamiltonian of a 2D quantum gas

Cheng Chin

An intriguing development in modern atomic physics research comes from the realization that at sufficiently low temperatures, the Hamiltonian of quantum gases can be easily engineered and programmed based on electromagnetic fields. The current state-of-the-art offers an intriguing prospect to gain full control of the Hamiltonian of a quantum many-body system to simulate novel quantum phenomena and implement quantum information processing.

Here we consider a generic Hamiltonian *H* of atoms confined in an optical lattice. It includes kinetic energy *K*, interaction energy *U* and potential energy *V*, given by

$$H = K + U + V = \sum_{<j,k>}(t_{j,k}a_j^{+}\, a_k + H.c.) + \sum_j U_j \frac{n_j(n_{j-1})}{2} - \sum_j \mu_j n_j,$$

where the summation goes over all sites in a 2D lattice, $t_{j,k}$ is the locally defined tunneling between neighboring sites, U_j is the locally defined interaction, and μ_j is the locally defined potential energy.

The full control of Hamiltonian, including all three terms, is based on a powerful toolbox that we will develop. In the following we will describe the ideas and how one employs and integrates them to gain control of the system on single atom level and in real time.

1. *Control of lattice potential: Holographic projection based on spatial light modulation*

The state-of-art in quantum control of cold atoms involves spatial light modulators, a modern tool to engineer arbitrary light pattern with high spatial and temporal resolution. An example is the Digital Micromirror Device (DMD), which contains millions of metallic mirrors. Each mirror is few microns in size and can be independently and fast switched. An application of the DMD is to holographically project an arbitrary lattice pattern to confine atoms. Such devices have been widely employed in recent cold atom experiments to generate quantum gas in a square well, optical lattice, ring-shape, and even random potentials. Here we summarize some of the results from our laboratory at the University of Chicago and ways to further improve its performance.

A holographically formed optical lattice is built site by site. It can be constructed based on various approaches: diffractive optical elements, high resolution liquid crystal modulators, or DMDs. All of the approaches generate very flexible lattice geometry, for example, square, triangular, honeycomb and even quasi-crystal lattices. DMDs, in particular, provide great flexibility compared to other devices with superior stability and reproducibility. It, however, also suffers from weak optical interference and requires fast electronics to program all mirrors.

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