Topical Review

Trapping ions and atoms optically

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Abstract
Isolating neutral and charged particles from the environment is essential in precision experiments. For decades, this has been achieved by trapping ions with radio-frequency (RF) fields and neutral particles with optical fields. Recently, the trapping of ions by interaction with light has been demonstrated. This might permit the advantages of optical trapping and ions to be combined. For example, we would benefit from superimposing optical traps to investigate ensembles of ions and atoms in the absence of any RF fields and from the versatile and scalable trapping geometries featured by optical lattices. In particular, ions provide individual addressability, and electronic and motional degrees of freedom that can be coherently controlled and detected via high-fidelity, state-dependent operations. Their long-range Coulomb interaction is significantly larger compared to those of neutral atoms and molecules. This enables ultra-cold interaction and the chemistry of trapped ions and atoms to be studied, as well as providing a novel platform for higher-dimensional experimental quantum simulations. The aim of this topical review is to present the current state of the art and to discuss the current challenges and prospects of the emerging field.

Keywords: trapping, cooling, quantum control

(Some figures may appear in colour only in the online journal)

Introduction

Trapping charged atoms in radio-frequency (RF) fields features deep trapping potentials of the order of \( 1 \text{ eV} \approx k_B \times 10^4 \text{ K} \) and related long lifetimes, as well as Coulomb interaction over a long range. For decades, trapped ions and advanced tools for their control have propelled many fields of research [1, 2]. For example, progress in the realm of quantum information processing has resulted in the unique control of the motional and electronic states of individual ions [3, 4], located in one-dimensional Coulomb crystals, that is, linear strings of up to 20 ions. Operational fidelities close to unity for state preparation, phonon-mediated interactions and detection allow the state of the art to be reached or set for a few particles in quantum metrology [5–7], quantum computation [8–11], as well as in analogue and digital quantum simulation [12–16].

However, trapping via RF fields is accompanied by inevitable side-effects such as RF-driven motion. This so-called micro-motion is superimposed on the secular motion of the ion within its time-averaged trapping potential and is undesirable or detrimental for several applications [6, 18–20]. In addition, scaling Coulomb crystals in size and dimension while preserving the level of individual control remains a demanding task [4, 8, 21]. For neutral particles, optical fields are a well-established technique for confinement in potential wells of the order of \( k_B \times 10^{-3} \text{ K} [22] \), featuring versatile trapping geometries scalable to large two- and three-dimensional lattices [23]. Combining the advantages of ions and optical traps has been achieved by a number of different approaches.

Using spatially overlapping optical fields to trap neutrals, and RF fields to trap charged atoms to study atom–ion interaction has led to seminal experiments in so-called hybrid traps [24]. In the temperature regime of tens of millikelvin, reactive collisions involving molecular ions have been studied [25, 26]. To reach even lower temperatures, RF-trapped ions have been immersed into clouds of ultra-cold atoms [27–30], such as Bose–Einstein condensates (see figure 1(a)).
Another approach is to provide the trapping of ions, replacing the confinement along the axis of a linear RF trap with a one-dimensional optical lattice. This permits the trapping potentials to be shaped locally while keeping the RF confinement for the radial degrees of freedom [33–36]. This approach has opened new perspectives, e.g. for the study of classical and quantum phase transitions in the context of friction [37–39].

The approach emphasized in this review focuses on trapping ions in optical fields and omitting any RF field. This has been achieved for the first time in a closely detuned optical dipole trap [40] in ultra-violet (UV) light, followed by a one-dimensional optical lattice [41]. Recently, the trapping of ions in a far-detuned optical trap (vis) has been reported [42]. Further improvements resulted in the lifetime of a Doppler-cooled ion reaching several seconds, exploiting enhanced control and a further detuned laser (NIR) [43].

The long lifetimes of ions in dipole traps, accompanied by long coherent times and low heating rates, are beneficial for reaching the regime of ultra-cold interaction in dilute atom–ion ensembles, and key for experimental quantum simulations in optical lattices with many ions—or ions and atoms—as anticipated in figures 1(b) and (c).

In the following, we aim to discuss the challenges and prospects of the field on the basis of two showcases:

1. In the field of ultra-cold chemistry: embedding optically trapped ions in quantum degenerate gases is predicted to allow temperatures that are four to five orders of magnitude below the current state of the art to be reached (see figure 2 and references [18, 19, 31]). This should permit a regime to be achieved where quantum effects are predicted to dominate: (i) in many-body physics, including the potential formation and dynamics of the mesoscopic clusters of atoms of a Bose–Einstein condensate, binding to the ‘impurity ion’ [44], as well as (ii) the subsequent two-particle s-wave collisions, which is the ultimate limit in ultra-cold chemistry.

2. In the field of analogue quantum simulations (AQS): optically trapping ions in lattices might provide a short-cut regarding the current lack of scalability in the size and dimension of the trapped ion systems. In addition, new classes of quantum simulations will become accessible, by combining optically trapped ions and atoms in common optical lattices (see figure 1 and references [15, 17]).

Methods

We want to summarize the fundamental questions on the general limitations and challenges of the optical trapping of ions, as well as the methodology required.

While preparation and detection remains provided by a conventional, linear RF trap, optical trapping is performed in the presence of electric stray and control fields, but in the absence of any RF field. The experiments so far have followed a common protocol [40], further detailed in the
sections below. An atom out of a thermal beam is resonantly photo-ionized and trapped in a linear Paul trap. The confinement is provided by RF fields for the radial degrees of freedom and by dc-fields along the axis (see figure 2). After the trapping and cooling of the ion, (1) the Doppler cooling laser is switched off, (2) the dipole trap laser is switched on, and (3), the RF potential is ramped down to zero. The dipole trap is kept on for the optical trapping duration. Afterwards, the sequence is reversed for the transfer back into the conventional Paul trap. If the CCD camera monitors the fluorescent light of the ion during Doppler cooling again, it reveals with near unity efficiency that the trapping attempt has been successful. Note that during the transfer between the different traps, all fields have to be considered simultaneously.

**Coupling of external fields to the charge monopole and the optically induced dipole**

We discuss the consequences of the charge monopole on the trapping characteristics within the optical trap, which relies on the optically induced dipole. This includes the ion’s dynamics during the intermittent exposure to the RF dc-optical potentials while being transferred between traps, and the potential ‘onset’ of differences in optically trapping ions compared to optically trapping atoms [22]. To the best of our knowledge, all the relevant aspects have been considered and elaborated on [45] and we have identified the main, technically remaining limitations: the stray electric fields. All the topics are briefly summarized in the following; our current solutions are listed, while their details can be found in the specified references. For the case of stray electric fields we present our current working solution in more detail in the following subsection.

(1) The effect of the light field directly interacting with the charge causes a residual, optically driven micro-motion [45]. Calculations show that this has a negligible impact since it remains further detuned by seven orders of magnitude compared to the RF. For an atom–ion ensemble, it is predicted to permit the pico-Kelvin regime to be reached.

(2) The impact of constant or slowly drifting stray electric fields on the charge disturbs the trapping conditions [46] and can shift the ion out of the shallow optical potential, independent of the temperature of the ion [47]. To permit the laser intensities to decrease and reduce the related off-resonant scattering and heating effects, the stray electric fields have to be further diminished (see below).

(3) The impact of the curvature of the dc-fields inevitably reduces the overall trapping potential by de-focusing [47], following Laplace’s equation [2]. These dc-fields are required in order to provide dc-confinement in some degrees of freedom, controlling curvatures (trapping frequencies) and the orientation of the principal axes [48], while allowing for additional diagnostics and control.

(4) The dynamics caused by switching optical and RF fields, e.g. to control the transfer of the ion between traps, can affect the stability of the individual traps and have consequences for the ion exposed to their intermittent overlap [41, 47]. On the one hand, the RF potentials should be switched sufficiently quickly to cross higher order resonances within the stability regime of the idealized quadrupole potential [49] without relevant energy transfer. On the other hand, they must be switched sufficiently slowly in comparison to the inverse of the relevant trapping frequencies to enable an adiabatic transfer. In addition, optical lattices might feature trapping frequencies of the order of half of the frequency of the RF drive, causing direct or parametric heating. Intermittent storage within a dipole trap and subsequent switching to the lattice in the absence of the RF turns out to be viable [41].

(5) The trapping conditions degrade if the frequent reloading of both species of choice is required. A higher background pressure reduces the lifetime and compromises stable conditions, either by lethal collisions,
enhanced by higher ion–atom cross sections compared to their neutral counter parts [50], or the non-deterministic near-crossing trajectories of residual ions tramping in the RF trap. Cleaning the trapping volume completely, e.g. by switching off the RF field while saving a single ion by an intermittent dipole trap turns out to be helpful. Ablative loading via a pulsed laser system can help to reduce this problem [51] accompanied by efficient photo-ionization [52]. Further improvement is anticipated following the concept of conveyor belts for single, sympathetically cooled molecular ions [53, 54], up to crystalline, three-dimensional beams of ions [55], as established in this context for atoms [29, 30, 56], passing differential pumping sections. Cleaner conditions can be further assisted by a cryogenic environment. These measures will also help to reduce the deposition of patch potentials, beneficial for decreasing the impact of the effects mentioned in (2) and below.

(6) The effect of technical noise outside the environment can be mitigated by efficient filtering—ideally down to a level where fluctuating patches on the surface of the electrode cause anomalous heating [4]. This is currently not a limiting factor for experiments, since these effects drop with $d^{-3}$, where $d$ represents the distance to the electrode. However, for even further reduced laser intensities and related trapping frequencies, these effects might again influence the ion when aiming for the lowest temperatures. Recently, methods for reducing anomalous heating by more than two orders of magnitude with either surface treatment [57–59] or cold electrode surfaces [60–62] have been reported. The fundamental limitation will be set by Johnson noise, related to the thermal motion of the electrons within the metal, decreasing with the decreasing temperature of the electrodes [58]. The heating due to beam pointing and the frequency/intensity jitter of the lasers involved should remain comparable to their effects on neutral atoms; however, the ensemble will remain prone to a mutual jitter of lasers within a bi-chromatic trap.

Compensation of stray fields exploiting the ion as the sensor

The state-of-the-art techniques for compensating stray electric fields has to be improved by two orders of magnitude, (1) to set the stage for the compensation of excess RF micro-motion in hybrid traps containing Li-atoms [18], and (2) to further improve optical trapping conditions in the future—for example, to permit optical trapping at substantially lower laser intensities [42].

We have to consider that trapped ions will be displaced by residual stray-fields. Optical trapping is possible for the maximal displacement of half of the beam waist, where Gaussian beams yield the steepest gradient and their maximal counter-acting force, respectively (see figure 3(a)). Note that optical forces acting on the ion can remain comparable to the trapping forces of the minimal RF confinement obtained just before the RF field is switched off, even though the total depth of the trapping potential shrinks by six to seven orders of magnitude. Our method of choice is based on minimizing the displacement of the ion while operating the RF trap [42], even though the RF drive is irrelevant after the RF trap has been switched off. This approach exploits the ion itself as a sensitive detector to identify displacements due to residual fields by switching the depth of the RF pseudo-potential between extremal amplitudes. Exploiting the tightly focused dipole beam itself, which is still strongly attenuated, still induces a differential dc-Stark shift. This alters the fluorescence rate of the ion depending on its position and relates it to the two stray-field-dependent positions for two different RF confinements. In addition, the method allows the overlap of the centres of the RF trap and the optical trap(s) to be optimized, minimizing heating during

Figure 3. Optical trapping potentials for $^{138}$Ba$^+$ (blue) and Rb (red) for different available laser powers within the bi-chromatic (1064 nm and 532 nm) dipole trap of given waists. (a) The 532 nm beam is responsible for trapping Ba$^+$ (493 nm) and leads to a defocusing effect in the bi-chromatic trap centre for Rb (780 nm), mainly stored by the 1064 nm wavelength, spatially separating the two species. (b) Increasing the IR power permits the compensation of the de-focusing effect and the spatial overlapping of the atoms and the ion in the center. Adjusting the relative laser power will allow the depth of the optical traps to be tuned individually, enabling the control of the evaporative and sympathetic cooling rates, for example. Preparing sufficiently low temperatures by side-band and sympathetic cooling might make common trapping within the NIR trap advantageous again.
the imperfect adiabatic transfer between the traps. Modulating the RF confinement and exploiting the lock-in techniques promise to further enhance the sensitivity.

**Protocol of optical trapping: RF trap for established preparation/cleaning and detection only**

The procedure for optically trapping a $^{24}\text{Mg}^+$ and $^{138}\text{Ba}^+$ ion within UV (280 nm) [40, 41], vis (532 nm) [42] and NIR (1064 nm) [43] dipole traps is identical. The direction of the $k$-vector has been varied, enclosing it between $45^\circ$ and $0^\circ$ on the $z$-axis of the linear trap (see figure 2), realized in three different apparatus [54, 63]. To load an ion into a dipole trap and to finally detect its optical trapping consists of the following steps:

1. Photo-ionizing an atom out of a thermal atomic beam, trapping it, Doppler-cooling it in a conventional RF trap and appropriately compensating for the stray fields.
2. Providing the dipole trap with a Gaussian laser beam focused onto the ion and switching off the RF drive of the Paul trap. From this time on, the ion is confined by the dipole trap in the directions perpendicular to the $k$-vector of the beam. The conventional dipole trap is assisted by dc-confinement along the axis of the linear trap, while the 1D optical lattices provided by retro-reflecting the beam confines the ion all optically. Loading might have to be assisted by an intermittent step (see issues of parametric heating mentioned above).
3. Switching on the RF drive again and verifying the presence of the ion via its fluorescence during Doppler-cooling. Ac-Stark shifts and the related optical potentials and forces depend on the wavelength of the dipole laser and the dedicated electronic state [22].

$^{24}\text{Mg}^+$, a red detuned UV dipole laser provides trapping in the $S_{1/2}$ ground state. The vis trap on $^{138}\text{Ba}^+$ provides trapping in the $S_{1/2}$, but anti-trapping in the $D_{3/2, 5/2}$ states. The latter can either become occupied by optical pumping or reached by off-resonant scattering, leading to a loss of the optically trapped ion. Recently, a re-pumping scheme was realized, allowing the $D_{3/2, 5/2}$ states to be de-populated during optical trapping, prolonging the lifetime of the ion by an
order of magnitude [43]. The NIR trap on $^{138}$Ba$^+$ provides trapping in the $S_{1/2}$ and in the $D_{3/2,5/2}$ states, with the latter still confined, but at trap depths reduced by $\sim 75\%$ [43].

We determine (i) the lifetime, (ii) the temperature, (iii) the heating rates and (iv) the scattering rates by measuring the optical trapping probability depending on different parameters. To access (i) we vary the duration of the trapping attempt, for (ii) we alter the optical trap depth and for (iii) we follow the protocol of the temperature measurement, however, adding a delay between the preparation and optical trapping. During this, delay trapping is still secured by RF fields, however, it incorporates the specific operation to investigate its impact. To derive (iv), we study the influence of re-pumping the lasers.

In addition, there is a huge variety of control, diagnostic and detection schemes, which are available from working on small numbers of ions in RF traps [4]. Methods, such as (sympathetic) cooling to the motional ground state [64], individual addressing [65], state detection with close to unit efficiency down to single-photon sensitivity [66], coherent state operations [5, 17], as well as vibrational spectroscopy with femto-second resolution on single molecular ions [53], are at hand already, still waiting to be exploited.

Results

Trapping the ions optically

In the year 2009, the optical trapping of a $^{24}$Mg$^+$ ion in the absence of any RF fields, was achieved (optical power $\sim 0.2$ W at a waist of $\sim 6.5 \, \mu$m), first in a single-beam dipole trap, superimposed by a static electric potential [40]. Subsequently, all optical trapping of the ion in an optical lattice (1D standing wave) has been demonstrated [41] for similar parameters. However, the lifetime of the ion remained limited to millisecond. This was due to off-resonant photon scattering out of the trapping laser field and the related photon recoil. At a recoil energy of $2E_{\text{recoil}} \approx 10 \, \mu$K and a scattering rate of 750 ms$^{-1}$, the ion is heated out of the comparatively shallow trapping potential at a depth of the order of 40 mK.

The one-dimensional pinning of ions in RF hybrid traps was reported in the year 2010 for $^{40}$Ca$^+$ [34] and in 2012 for $^{174}$Yb$^+$ [36]. Radially, the confinement of the ion(s) along one axis was still achieved by an active linear RF trap, however, it overlapped the axis of the standing wave within the optical cavity. Side-band cooling close to the motional ground state has also been achieved within these novel hybrid traps [36].

In 2014, the purely optical confinement of a $^{138}$Ba$^+$ ion within a far-detuned dipole trap was demonstrated (optical power of $\sim 10$ W at a waist of $\sim 4 \, \mu$m). This allowed recoil heating to be reduced by four orders of magnitude; however, the lifetime remained limited to milliseconds. This is still due to the off-resonant scattering rate: indeed, the latter is strongly reduced by three orders of magnitude, but remains responsible for optical pumping into metastable electronic states of Ba$^+$, featuring different ac-Stark shifts and repelling forces induced by the vis dipole laser.

Still, the lifetime is sufficient to immerse Ba$^+$ ions into an ensemble of ultra-cold atoms within a common dipole trap and to investigate sympathetic cooling already. To permit efficiently enhanced life and coherence times in dipole traps and optical lattices, following the receipt of trapped neutral atoms, the detuning as well as the laser power has been increased [22]. In 2016, the trapping of a Ba$^+$ ion within an IR dipole trap was achieved [43]. This is the key prerequisite to permitting the confinement of ultracold atoms and ions in a common (bi-chromatic) optical trap (see figure 3).

Considering the compensation of stray electric fields, we have currently reached the level of 1 mV m$^{-1}$ at the position of the ion. This level permits the intensity of the lasers to be lowered and is sufficient to address and test predictions of the suitability of Li for reaching the quantum regime in hybrid traps [18].

Discussion

The aim of this section is to discuss the significance of the results reported above to help circumvent the fundamental limitations or substantial challenges in applications by combining the advantages of optical trapping and ions. First, we discuss the requirements and prospects of optical trapping in the regime of temperatures directly reached by Doppler-cooling. Second, we dwell on the improvement of our approach in the context of aiming at reaching the regime of ultra-low temperatures. The related prospects for some applications, illustrated in figure 1, will be described in the next section.

To increase the lifetime, lower laser intensities and related scattering rates are beneficial. Currently, deep optical traps are still required to permit ions to be trapped at comparatively high initial temperatures. A promising option for reducing the residual loss is to choose an ion species with a reduced branching ratio into metastable states, or even featuring a closed transition only. For some applications, e.g. those dependent on a larger amount of optically trapped ions, it might be sufficient to increase the rate of re-pumping by stroboscopically alternating the laser exposure at a rate that is much higher than the inverse of the secular frequencies. Still, residual scattering compromises the longer coherence times.

Coulomb crystals in optical traps

To illustrate the protocol for entering the regime of ultra-cold atom–ion ensembles, we select the combination of a $^{138}$Ba$^+$ with two atomic species of extremely different masses, $^{87}$Rb and $^{6}Li$, here focusing on Rb. Long lifetimes are indispensable for scaling to a larger number of ions to investigate the multiple ions trapped in the optical potential(s). For
example, the study of Coulomb crystals and structural phase transitions to more dimensional structures at Doppler temperatures, has been well-established and exploited in RF traps [67, 68]. However, more dimensional Coulomb crystals in RF traps experience the even more enhanced impact of the RF field on the ions, since the ions are intrinsically displaced from the RF-free axis. In this context, the state dependency of optical trapping potentials and the available coherent control of electronic states can be exploited to follow intriguing proposals on structural phase transitions [69–72] and related quantum effects. Optionally, embedding sympathetically cooled (molecular) ions or even sympathetically cooled, positively charged ions, which are sufficiently close, but spatially separated from ions of negative charge will enrich prospects.

**Cooling atom–ion ensembles into the quantum regime**

To provide the required bath of ultra-cold atoms, we follow established procedures [73].

(a) Realizing an all optical, bi-chromatic trap for $^{138}$Ba$^+$ ions and $^{87}$Rb atoms: the loading of Rb atoms into an MOT (typically $2 \times 10^8$ atoms ($\sim 10^{11} \text{ cm}^{-3}$ at 150 $\mu$K–50 $\mu$K after an optical molasses, with a lifetime of $>10 s$), followed by an all-optical BEC ($4 \times 10^4$ atoms after 3 s of loading and evaporative cooling to 50 nK temperatures). It has been demonstrated that Ba$^+$ ions can become trapped in vis and NIR dipole traps [43]. Combining the two provides a bi-chromatic dipole trap that permits the confinement of the Rb atoms to be controlled separately (see figure 3). Specifically, this permits the dependent (de)focusing of the species to be induced, and thus allows additional control of the spatial overlap and the density of the atomic ensemble in the vicinity of the ion. The example shown in figure 3(a) depicts the deep confinement of earth alkali ions in the centre of the bi-chromatic trap, while a dedicated choice of beam parameters provides a Mexican-hat-like potential for the alkaline atoms due to the vis laser remaining detuned to the blue of their relevant transitions. Simpler choices, such as the confinement of the atom–ion ensemble by the NIR laser alone, would provide deeper confinement for the atoms; however, it might also compromise sympathetic cooling during evaporation of the atoms.

To reduce loss mechanisms while sympathetically cooling the ion embedded in the cold atomic ensemble, e.g. due to three-body collisions [74] (see also figure 4), might require initially reduced atomic densities and related extended periods of elastic atom–ion interaction. In this context, it might become essential for the measured upper bound of the heating rate of an ion in the presence of trapping and ambient fields to remain sufficiently low, for example, in comparison to the predicted sympathetic cooling rates, as estimated in [75]. Reaching sufficiently low temperatures at the first stage will allow the option of trapping the ensembles in the NIR trap. Fully exploiting the current level of stray field compensation ($E \approx 0.001 \text{ V m}^{-1}$) might permit substantially lower laser intensities [42].

(b) Sympathetically cooling $^{138}$Ba$^+$ by $^{87}$Rb (BEC) down to 100 nK: the atomic system is predicted by theory to be suitable for sympathetically cooling the ion–atom ensemble to the temperature of the atomic bath on the time scale of milliseconds [75].

Several methods are at hand to measure the rate of sympathetic cooling and the final temperature, such as deriving the energy distribution of the ion by fitting optical trapping probabilities assuming the energy cutoff model [47], sideband diagnosis [4, 30] and analyzing the loss rate of the atoms, as demonstrated in the hybrid traps already [56].

(c) Sympathetically cooling $^{138}$Ba$^+$ by $^4$Li and $^7$Li: a comparison of trapping via RF versus optical fields. It should become possible to elucidate the prospects of Li atoms as (i) sympathetic coolant, which is advantageous since their small mass makes them highly efficient; (ii) a collision partner, offering different isotopes of bosonic and fermionic nature; (iii) insensitive to charge transfer, since the relevant inelastic reactions in the Li-Ba$^+$ system are expected to remain endothermic (Li and Ba$^+$ forming the ground state); and (iv) remaining currently the only atomic candidate species not fundamentally excluded from exploring and exploiting the ultra-cold regime in hybrid traps. In this context, it is worth mentioning that it has recently been argued that the first few collisions might also get probed in RF traps for a wide range of species [30].

**Conclusion**

In this section, we aim to further highlight the novelty of the approach by concluding with plans for future work.

**Ultra-cold interaction—quantum many-body effects**

Optical trapping should enable the exploration and direct observation of many-body processes in the atomic BEC-ion system within the ultra-cold regime. This includes, for example, the test of the related predictions on the rapid and efficient formation of a metastable and mesoscopic molecular ion, and binding of the order of hundreds of atoms of the BEC within the common ion–atom $r^{-4}$-potential (see figure 4 [4] and [44]). It has to be noted that the related atomic densities within these objects at the predicted sub-micrometre diameter would rise to extremely high values. That is, the dynamics might be strongly affected by three-body collisions and related losses [74], requiring a description beyond the mean field theory that the predictions are currently based on. Additional mutual dipolar repulsion of the polarized atoms or even active control via simultaneous atom–atom and the predicted atom–ion Feshbach resonances might be considered [19, 76]. The system might allow the characteristics and related dynamics of the ion–atom system to be revealed during cooling to the nano-Kelvin regime, exploiting tools to
control the parameters and detecting the observables of the many-body system directly. Gaining an insight into the underlying processes, as well as into the prospects for exploring and exploiting the control might relate these results to solid state/cluster physics; relevant, for example, for processes in condensed matter systems and liquid helium where so-called snowballs and electron-bubbles have been observed [77]. There are substantial advantages of the atomic BEC-ion system. For example, the low atomic density should permit comparatively clean experiments, while winning established techniques from the field of quantum optics permits highly efficient detection and control for the novel system. One of the key features of a heterogeneous approach is the ability to distinguish the Ba\(^+\) from the atomic Rb-BEC, thus eliminating the resonant charge transfer. Potential tools include:

(a) Measuring the secular frequency, i.e. the effective mass of the immersed ion. Classical vibrational spectroscopy [48] will allow a direct comparison of the secular frequency of the ion, when it is bare and immersed into ultra-cold atoms. Any interaction, especially the potential binding of atoms to the ion, will affect the oscillation frequency of the ion in the optical trap. Thus, measuring the altered frequency can be interpreted as observing a dressed ion featuring an effective mass related to the amount of bound atoms, e.g. via the resonant excitation and the related enhanced loss rate of atoms out of the surrounding ensemble.

(b) Measuring motional excitation on the quantum level: phonon-spectroscopy via two-photon-stimulated Raman transitions can be exploited (i) to implement side-band cooling to the motional ground state of Ba\(^+\), e.g. for the initial state preparation, and (ii) to measure the population of the quantized motional states, permitting direct measurements of the temperature and energy distribution of the ion, respectively [30]. Additionally, the related motional control can be extended to the predicted ion–atom cluster to (iii) gain external control on the rising and falling rates of the atomic population in the bound states. For specific energies/detunings, and as the atoms surrounding the ion drop deeper into the ‘ionic well’, the remaining BEC atoms would gain energy and be ejected from the trap, leading to quantized atom loss rates for discrete laser detunings, potentially assisted by modulation of the trapping potential. Thus, implementing (iii) could permit the binding energy, chemical potential and energy difference between bound states to be to spectroscopically resolved [44]. Additionally, driving the transitions at dedicated Rabi-rates might permit the timescales for the formation of the cluster to be revealed, as well as measuring and controlling the internal state dynamics on their path from an originally metastable state (all bound atoms in the highest excited state) towards its deeper bound states, and extract the dependence on relevant parameters of the system, such as its finite size and temperature.

(c) Detection of the interaction range of polarization via EIT: recently, it has been shown that EIT is suitable for imaging the blockaded Rydberg sphere in the cold atomic samples [78], permitting the non-destructive detection of the Rydberg excitations. The interaction between the two Rydberg atoms is reported to become sufficiently strong to shift the relevant energy levels out of resonance. Illuminating the atoms by a pair of EIT lasers reveals a shift of levels, breaking the former condition for transparency, causing the region affected to become opaque again. A similar approach should be applicable in atom–ion systems: in the region surrounding the ion, the atoms experience a mutual dipole–dipole interaction and the polarization interaction due to the ion might shift the relevant levels sufficiently to break the EIT condition, hence leading to a way of imaging the location and size of the related cluster. Combined with the method described in (a), the atomic density within the ion–atom ensemble might become accessible.

(d) Exploiting the sensitivity of the ‘ion-impurity’ to external fields: depending on the success of the methodology described above, the control on the BEC might be extended itself, using the ion as an inherent impurity, precisely addressable by external fields. Applications might include (i) creating and controlling rotational excitations (vortices) within the BEC, (ii) controlling the spatial position of the BEC by electrostatic forces and altering the trapping conditions, and (iii) immersing more than one ion into the BEC causing the potential partial shielding of their charges and mutually reduced repulsion, e.g. to further extend (i) and (ii).

Ultra-cold chemistry—reactive collisions

Depending on the dynamics occurring on the way towards the ultra-cold regime, two-particle \(s\)-wave collisions can be reached. The ultimate limit in ultra-cold chemistry might become accessible in fundamentally different ensembles. Examples include: (1) the Ba\(^+\) ion and Rb, which are fundamentally out of reach for hybrid traps. (2) \(^{138}\)Ba\(^+\) and \(^6\)Li, which are \textit{a priori} not excluded for hybrid traps, assuming a sufficient level of stray-field compensation. Here, we briefly discuss the Ba\(^+\)-Rb system (see figure 5). The collision process between the Ba\(^+\)(\(2S\)) ion and the Rb\((2S)\) atom involves elastic scattering (EL) between the ion and the atom, and two types of inelastic events: a charge transfer (CT) and radiative association (RA). Elastic collisions will lead to the initial energy transfer from the ion to the cold atom(s), that is, sympathetic cooling of the ion and the subsequent escape of the atom(s) from the trap. This process will also yield ultra-cold ions in the first place, if the cross section for the elastic scattering is much larger than that for the inelastic events (predicted to be fulfilled for Rb and Ba\(^+\) [75]). Molecular states of the (BaRb)\(^+\) molecule, corresponding to the Ba\(^+\)(\(2S\)) + Rb\((2S)\) dissociation limit, are excited states of the molecular ion (the ground state corresponds to the Ba\((2S)\) + Rb\((2S)\) asymptote, lying approximately 8344 cm\(^{-1}\) below the Ba\(^+\)(\(2S\)) + Rb\((2S)\)
asymptote). The collision between the Ba$^{+}(^2S)$ ion and the Rb$^2$(S) atom can lead to the formation of the bound (BaRb)$^+$ molecular ion in its electronic ground state via RA. The continuum wave function of the singlet and triplet manifold, corresponding to the Ba$^{+}(^2S) +$ Rb$^2$(S) dissociation limit, is connected to (several) bound ro-vibrational levels of the ground electronic state through the electric dipole operator. A different inelastic mechanism, which may occur in the collision between the Rb$^2$(S) atom and the Ba$^{+}(^2S)$ ion, involves the CT of the electron from the Rb$^2$(S) to the latter. Finally, a free Ba$^1$(S) atom and a Rb$^1$(S) ion will arise. The continuum wave function of the excited triplet and singlet manifold is again the electric dipole connected to the ground electronic state, but this time to the ro-vibrational continuum.

Close collaboration with theory might allow the relevant processes to be mapped out as a function of the experimental conditions (e.g. energy/temperature, electric/magnetic fields, preparation of internal states of atoms/ions). It is worth emphasizing that optical fields can influence the formation and dissociation of molecules, respectively. Dependent on the wavelength, they might assist the formation of molecules by radiative association or transfer population into dissociative channels [25, 79]. Experimental data is required for understanding and ultimately controlling the behaviour of mixed atom–ion systems in the quantum regime.

**Experimental quantum simulations—designing quantum many-body effects**

We sketch how the field of analogue quantum simulations (AQS) might be enriched by optically trapped ions and atoms in optical lattices, originally considered for the field of QIP [80]. Optical lattices can be further stabilized and enhanced by optical cavities in more dimensions while benefiting from the coordinated choice of magic wavelengths [81] and state-dependent potentials [40]. For a more detailed and general overview in the context of our proposal, please refer to [16, 17, 63, 82–84] and the references therein. However, AQSs based on atoms and ions are already appealing in the presence of RF fields. The possibility of studying dynamics from Peierls transitions [85] to friction models with a very high degree of control is intriguing [37–39]. One option is to tailor non-harmonic potentials by a combination of the optical lattice potential and RF trap confinement, as suggested in [86], here, to study quantum heat engines, as well as motors and ratchets in such potentials, while considering quantum tunnelling.

Realizing the proposal of Richard Feynman, that is, running AQSs of mesoscopic size, is predicted to open new frontiers of science by studying high-energy physics, cosmology, atomic physics, quantum chemistry and even biology. With an envisioned size of only tens of ions/atoms/ spins, we can already perform useful AQSs, beyond the scope of classical computation [16, 87, 88]. In this context, we propose to exploit the major advantage of an array of ions compared to atoms in an optical lattice, that is, that the effective interactions are long-range, since they are mediated by the Coulomb force. Furthermore, we aim to circumvent at a stroke the major disadvantage of the ionic approach: its current lack of scalability in size and dimension. In addition, new classes of AQS will become accessible, by combining optically trapped ions and atoms in common optical lattices. It might be possible, for example, to study atoms in a completely occupied lattice, enriched by a small density of ions, sharing electrons by tunnelling, causing highly entangled states of the compound system featuring quantum dynamics governed by the Bose–Hubbard Hamiltonian. Further scaled AQSs would not only provide new results that cannot be predicted otherwise or classically simulated, but would also allow for the test of various models, required for substantially deepening our understanding of complex quantum dynamics.

Here, the proposed scaling in optical lattices might feature a controllable version of magnified lattice structures, providing clean control of otherwise unaccessible quantum effects in solids and possibly being used to study problems in condensed matter physics, such as correlated electrons or quantum magnetism, high-Tc superconductors, quantum Hall ferromagnets, ferroelectrics etc. Their experimental simulation would allow quantum phase transitions to be observed and analysed.

This review presents complementary approaches, identifying intriguing and challenging problems related to the optical trapping of ions as well as early experiments. Currently, the field is driven by rapid development and active research. Therefore, the larger picture is in no way complete, and we envision that the most exciting developments, and most importantly the related results, will provide a deeper insight into complex quantum behaviour in the (near) future.

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