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Electronics of an ion trap with integrated time-of-flight mass spectrometer

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ABSTRACT

Recently, we reported an ion trap experiment with an integrated time-of-flight mass spectrometer (TOFMS) [1] focusing on the improvement of mass resolution and detection limit due to sample preparation at millikelvin temperatures. The system utilizes a radio-frequency (RF) ion trap with asymmetric drive for storing and manipulating laser-cooled ions and features radial extraction into a compact 275 mm long TOF drift tube. The mass resolution exceeds $m/\Delta m = 500$, which provides isotopic resolution over the whole mass range of interest in current experiments and constitutes an improvement of almost an order of magnitude over other implementations. In this article, we discuss the experimental implementation in detail, which is comprised of newly developed drive electronics for generating the required voltages to operate RF trap and TOFMS, as well as control electronics for regulating RF outputs and synchronizing the TOFMS extraction.

1. Introduction

Experiments with molecular ions in radio-frequency (RF) ion traps have rapidly evolved in physics and chemistry in recent years. Such experiments focus on the production of molecules [2]; their cooling [3–8]; reactions of trapped ions with (untrapped) neutral reactants [9–12]; spectroscopy of molecular ions [13–17]; and precision measurements [18]. As opposed to neutral molecules, molecular ions allow for easy trapping and, optionally, sympathetic cooling of their translational degrees of freedom with co-trapped, laser-cooled atomic ions [19–21]. Since ion trapping is largely species independent, it is important to have a robust means to identify the trapped ions. This identification can be used to deduce reaction properties, such as reaction rates or branching ratios, or for destructive spectroscopy techniques involving e.g. photodissociation.

Closely related are experimental efforts with hybrid atom–ion traps [22–26]. Their implementation typically involves an RF ion trap for confining ions, which are overlapped with a cold cloud of atoms [22,23] or a Bose–Einstein condensate [27,28]. All-optical hybrid traps for atoms and ions are also in development, in which the RF trap can be turned off during certain experimental sequences [29–32]. A chief application of these systems is the study of cold/ultra-cold collisions and reactions of ions and atoms [33–40]. Conclusions on the reaction mechanisms can be drawn by trapping and, again, subsequently analyzing charged reaction products.

Mass spectrometry (MS) constitutes a powerful and straightforward way for the analyses of product ion samples in such experiments. While mass spectrometers with resolutions exceeding $m/\Delta m = 100,000$ are commercially available [41], such systems are usually bulky, expensive and difficult to integrate in experiments with cold ions and atoms. Hence, various techniques have been used to allow for discriminating different ions species in such experiments. These include mass filtering [42]; resonant excitation of the secular ion motion [20,43,44]; laser-induced fluorescence techniques [5,9,45–47]; or integrated time-of-flight mass spectrometers (TOFMSs) [1,12,14,15,18]. The former techniques are applicable without changes to the vacuum systems, but complicated due to nonlinear resonances of the RF trap [48], complex interpretation of the resulting spectra, demanding requirements on laser cooling including formation of ion Coulomb crystals, and/or the required molecular dynamics simulations. This is in particular true, if the sample contains a variety of potentially unknown ion species. As an alternative, integrated TOFMSs have proven to be unambiguous, be conceptually simple, be widely applicable, and provide a relatively high, sometimes isotopic, mass resolution.

An early implementation of an RF trap with integrated TOFMS is given in Ref. [14] and reaches mass resolutions of typically $m/\Delta m \sim 50$. The linear RF trap is operated symmetrically (with RF voltages of opposite sign at neighboring electrodes) using two center-tapped RF transformers. Pulsed application of slightly different high voltages (HVs) to the center taps of the transformers

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creates the two-stage electric field of a Wiley–McLaren TOFMS [49] and extracts ions radially [50,51] into a TOF drift tube. The radial extraction of this implementation has the advantage of a more compressed sample compared to an extraction along the axis of the RF trap, but sacrifices some of the gain in mass resolution due to the presence of RF ringing during the extraction. This system has been used to perform photo-dissociation spectroscopy of $BaCl^+$ [14], $SrCl^+$ [16], and $DyCl^+$ [17].

A later TOFMS implementation using a six-rod quadrupole RF trap with radial extraction is described in Ref. [18] and has been used for spectroscopy of HfF^+. The RF trap is driven at an exceptionally low drive frequency of about 50 kHz, such that drive voltages are generated without resonant enhancement which facilitates the application of the TOF extraction voltages. Although the six-rod RF trap has a different motivation in this system, such a trap geometry has the potential advantage of being able to use separate electrodes for RF and HV: while two opposing rods can be driven with RF, HVs can be applied to the other four rods and ions are extracted through a gap between two neighboring HV electrodes. A drawback for certain applications would be the reduced optical access for establishing, for example, an atom trap.

Another TOFMS implementation with axial extraction has been used to perform spectroscopy of AlH^+ [15]. While the mass resolution is limited, the implementation is appealing because of its simplicity and the separation of RF and HV electrodes.

Recently, a TOFMS with radial extraction has been demonstrated [12], in which the RF trap is operated with digital HV pulses instead of sinusoidal voltages [52,53]. This concept appears compelling, because the absence of RF voltages prevents the associated ringing and digital HV pulses can be directly reused for extraction into the TOFMS, however, the mass resolution in the given implementation remains $m/\Delta m \leq 90$. Further, the digital drive leads to enhanced micromotion and increased requirements on phase matching between different electrodes, which is disadvantageous during experimental cycles requiring cold ion samples.

In 2014, we demonstrated an RF trap with integrated TOFMS [1], which is loosely based on Refs. [54,14]. The TOFMS has a significantly higher mass resolution ($m/\Delta m > 500$) than other implementations. The RF trap is operated asymmetrically and can be actively damped during the application of the HV extraction pulses to prevent ringing. The basic setup and the effect of laser cooling on mass spectrometry have been sketched in Ref. [1]; here, we focus on the technical details.

In the following, we first explain the electronics for the RF trap/TOFMS in Section 2. This section is subdivided into an overview of the experimental apparatus (Section 2.1), RF trap and TOFMS design considerations (Section 2.2), the description of drive units generating the RF voltages and HVs (Section 2.3) and a control unit (Section 2.4), and remarks on the wiring of the RF trap and measuring of the voltages (Section 2.5). Subsequently, in Section 3, we conclude with a brief discussion of the performance of the system (Section 3.1) and potential future improvements (Section 3.2).

2. Experimental implementation

2.1. Overview

The apparatus consists of a segmented linear RF trap, and a basic, Wiley–McLaren [49] type TOFMS (see Fig. 1). More details and a three-dimensional rendering of the relevant components are given in Ref. [1]. Briefly, the RF trap is driven asymmetrically with one pair of diagonally opposing electrodes at RF voltage (amplitude $V_{RF} = V_0$) and the other pair at RF ground ($V_{RF} = 0$). We can choose between a drive frequency Ω of either $\Omega_< \approx 2\pi \times 720$ kHz or $\Omega_> \approx 2\pi \times 1.8$ MHz depending on the pair of electrodes being driven and reach RF amplitudes of up to $V_0 \approx 750$ V.

For the extraction into the TOF drift tube, the RF voltages are quickly turned off. Subsequently, the electrodes are pulsed to DC HVs U_{HV} with a 10–90% rise time of ≈250 ns. The HV is applied such that a two-stage electric field is established [49], which radially extracts the cold atoms and molecules from the RF trap into the TOFMS [50,51]. This is accomplished by applying a slightly lower HV to the electrodes which are closer to the TOFMS ($U_{HV} = U_1 = 1.2$ kV) than to the ones that are farther ($U_{HV} = U_2 = 1.4$ kV).

This scheme leads to a noticeable complication: While the same RF voltage V_{RF} is required on diagonally opposing electrodes for trapping, different U_{HV} must be applied to these electrodes for extraction into the TOFMS. In total, four different configurations of voltages (V_{RF} ; U_{HV}) must be generated: (0 ; U_1), (0 ; U_2), (V_0 ; U_1), and (V_0 ; U_2). Additionally, different low-voltage DC voltages U_{DC} need to be superimposed with V_{RF} on some segments to compensate micromotion and provide axial confinement.

The developed circuit, referred to as the drive unit (see Section 2.3) in what follows, generates one triplet of voltages (V_{RF} ; U_{HV} ; U_{DC}). We typically drive each segment of the RF trap

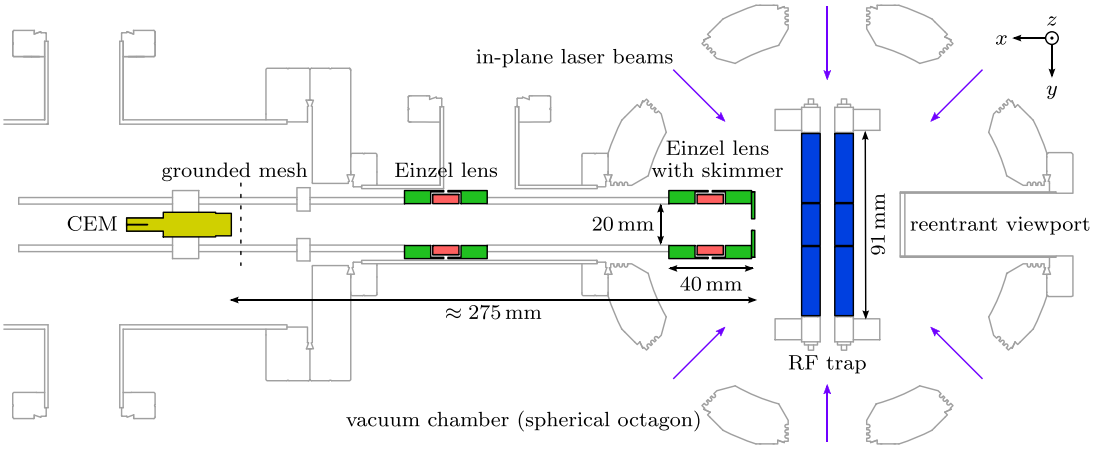

Fig. 1. Schematic of the vacuum apparatus (top view). The linear segmented RF trap has cylindrical electrodes with a field radius of $R_0 = 6.85$ mm and an electrode diameter of 9 mm. The TOF drift tube is aligned perpendicularly to the axis of the RF trap to enable the radial extraction. Two Einzel lenses (red/green), one at the entrance of the drift tube and one roughly in the middle of the drift tube, focus the ions onto a channel electron multiplier (CEM, yellow), which is shielded by a stainless steel mesh (transmission ~3/4). The first Einzel lens has an additional skimmer with a ≈6 mm diameter aperture (also green). Laser access for cooling of ions in the RF trap and an optionally overlapped magneto-optical trap for calcium atoms is possible from six in-plane directions and additional out-of-plane directions (not shown). The mounting structures and vacuum chamber (partially shown; gray lines) as well as the outer electrodes of the Einzel lenses (green) are grounded. The assembly is held under vacuum at a pressure of $\approx 10^{-9}$ mbar.