Studying Charge Exchange in a Hybrid Ion-Neutral Trap

Jonathan Kwolek

December 13, 2017

Abstract

Ion-neutral interactions are of great interest to researchers because of their astrophysical and spectroscopic implications. Ion-neutral interactions are intermediate range ($\sim 1/r^4$), and generally have large cross sections and easily measurable rates. The UCONN hybrid trap, a combination of a neutral and ion trap, is an excellent tool for studying these ion-neutral interactions. Quantum control in our neutral trap allows us to differentiate interactions by quantum state, and measure specific channels. Here, we propose an experiment to study the quantum state characteristics of a MOT, as well as an experiment to measure different rate constants for ion-neutral interactions in a hybrid trap.

1 Introduction

Hybrid traps enable the study of cold ion-neutral systems, which have far reaching implications in the world of physics. The ion-neutral interaction potential is intermediate range ($V \propto 1/r^4$) compared to ion-ion (Coulomb: $V \propto 1/R$) or neutral-neutral (van der Waals: $V \propto 1/r^6$) interactions. The size of these interactions are defined by the cross section. In the high energy limit, the classical Langevin cross section for ion-neutral interactions $\sigma \propto E^{-1/2} \propto \langle \mathbf{v} \rangle^{-1}$ becomes proportional to the inverse of velocity or $1/\sqrt{T}$, where T is temperature [1]. Because the ion-neutral collisional cross sections are much higher than neutral-neutral, it is easier to measure their reactions with low density traps. Conversely, since ion-neutral interactions are much shorter range than ion-ion interactions, ion-neutral interactions can be used to study interesting phenomena like internal state cooling of molecular ions [2, 3]. Today, there are many traps which allow us to obtain cold and ultracold temperatures for both atoms and ions, enabling us to study these interactions. Despite these interesting possibilities, the cold-ultracold ion-neutral interaction regime is largely unexplored experimentally.

In order to experimentally explore ion-neutral interactions, we must first trap neutrals and ions together. The neutral trap we use is called a Magneto-Optical Trap (MOT), first proposed in 1987 [4]. A MOT consists of near-resonance lasers with a specially oriented magnetic gradient, and can be used to achieve ultracold temperatures on the order of 10^{-4}K. This, in conjunction with laser or collisional cooling of the ions will allow us to reach the ultracold atom-ion interaction regime. Using a MOT as our neutral trap has the advantage of allowing control of the quantum states of the atoms in the trap. A MOT can be made with any alkali, many alkaline earth atoms, as well as some molecules. In the UCONN lab, we specifically use sodium.

Sodium MOTs have the advantage of using visible lasers, while also having a much more closely spaced level structure than the typical rubidium MOT. However, despite the fact that MOT's have been used since the late 1980's, there is still some disagreement about certain characteristic behaviors of the atoms in the trap. Specific to our experiment, we are concerned with the excited state fraction (f_e) in our MOT. Some reactions, such as charge exchange, occur predominantly when the neutral atom is in the excited state, so the reaction rate depends on f_e. Surprisingly, f_e has only been directly measured for MOTs of the two most common isotopes of rubidium [5, 6]. These experiments found that the simple two-level model has some predictive power when using a fitted effective saturation intensity instead of the theoretical value, however this model only works for a limited range of laser intensities. This is because rubidium is not a two-level atom, but in fact has other excited state hyperfine levels that the laser can accidentally excite, creating an effective loss mechanism out of the two-level system. Compared to sodium however, this process is much less likely due to the fact that the upper state hyperfine splitting is larger in rubidium (~ 5 times larger). Sodium also has a linewidth ~ 1.6 times that of rubidium, which will increase the loss rate. Because of these factors, we predict that we will see an even stronger deviation from the two-level model in sodium. Since we want to measure reaction rates that distinguish between quantum states of the reactants, we must gain a good understanding of the excited state fraction in our MOT.

The ion of our ion-neutral interaction must be co-trapped in the same space as the MOT in order to observe interactions. To do this, we use a linear r.f Paul ion trap (LPT). The Paul trap can be used on both large and small scales, and even to trap ions indefinitely [7]. This is because the typical trap depth (energy of the ion which the trap can contain) is $\sim$1000K. In contrast, a MOT has a trap depth around $\sim$1K. Historically, Paul traps have also been used in spectroscopy [8, 9], atomic clocks [10, 11], and can be very useful in studies of quantum information [12, 13, 14]. One reason we chose a linear Paul trap was that there is a nodal line for the ions where the micromotion is zero, and cold collisions with ions on this line can be studied.

With our colocated ion and neutral trap, we create what is called a hybrid trap. The hybrid trap enables cotrapping of atoms and ions in a common region, in order to study the long range ion-neutral interactions. The original hybrid trap was proposed by my advisor, W. Smith in 2003 [3]. Six years later, the first experiment was conducted by A. Grier and V. Vuletić at MIT in 2009. Since then, the field has exploded, with many labs currently using hybrid traps across the world. While a hybrid trap is typcally made with a Paul trap for the ions, the methods for cotrapping neutrals varies. Many groups including our own use MOTs [15, 16, 17, 18], however in order to achieve colder temperatures, some groups require a BEC [19, 20, 21, 22, 23, 24] or optical dipole trap [25]. Ultimately, the hybrid trap enables us to precisely measure medium range ion-neutral interactions, which have much higher cross sections and rates than the shorter
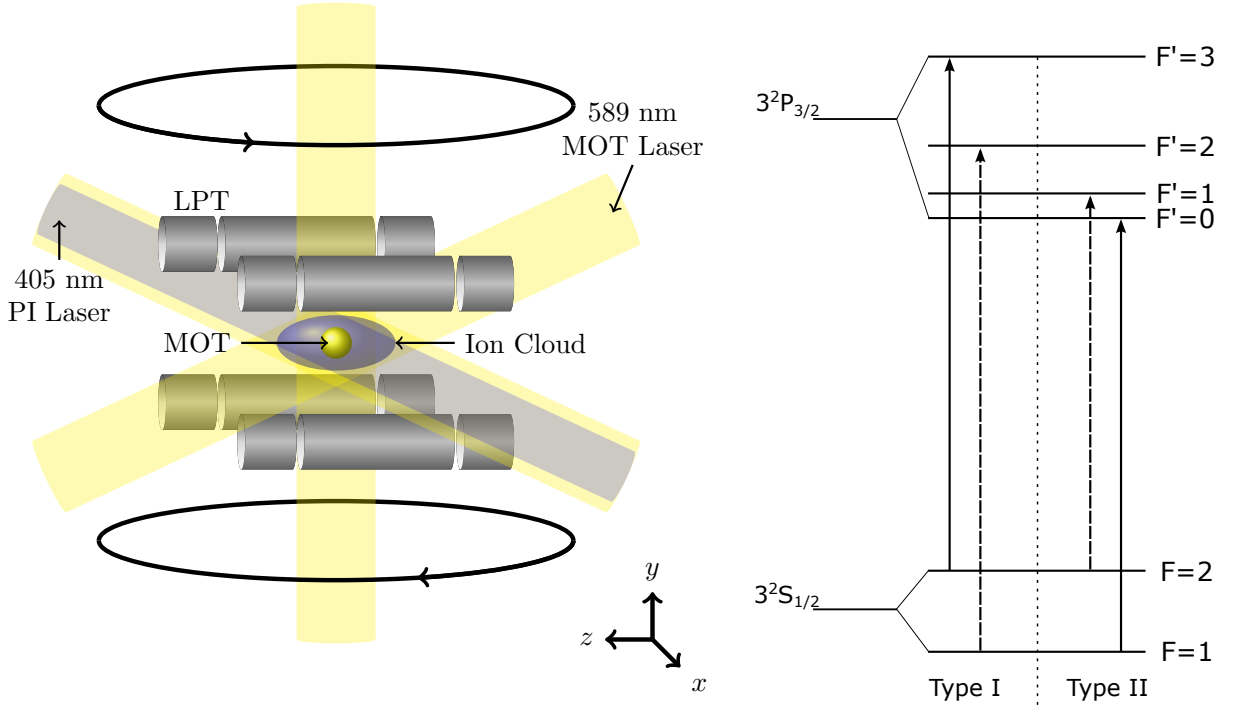
Figure 1: The hybrid trap consists of a colocated MOT and LPT. The MOT is made from 3 retroreflected 589 beams, which pump the sodium on the cooling and repump transitions (shown on the right as solid and dashed respectively for Type I and II). The magnetic coils in an anti-Helmholz configuration create a magnetic field which gives an appropriate dependance on the light forces to conservatively trap. The 405 nm laser is used to ionize sodium through REMPI, though depending on the experiment it can be replaced with 397nm, 866nm, 423nm and 375nm lasers (cooling and repumping of calcium ions, and excitation and ionization of neutral calcium). The LPT consists of 4 rods with r.f. applied as well as 8 d.c. end caps. This traps the ion cloud in the same space as the MOT.

range neutral-neutral interactions [26].

The proposal is organized as follows. First I will detail the UCONN hybrid trap, including our trapping methods and their benefits. I will then briefly discuss some recent work, and present background information about the charge exchange mechanisms as well as the methodology and intricacies of using a MOT. Finally, I will discuss the proposed research, including the direct measurement of f_e, as well as the further investigation and expanding upon charge exchange reactions previously discovered by our group.

2 Background

2.1 Hybrid Trap

A hybrid trap, first proposed by W. Smith in 2003 [3], is designed to study interactions between neutral atoms and ions. Since these reactions have relatively large collisional cross sections ($\sim 10^6$ a.u.), they can
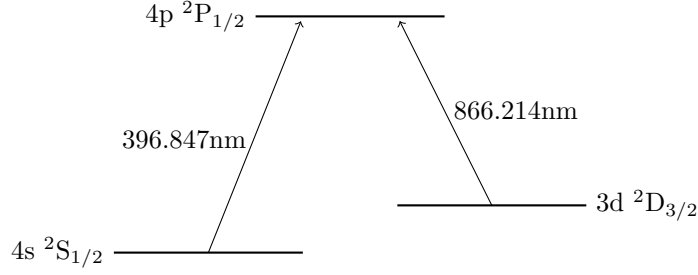
Figure 2: The low electronic energy levels of Ca^+ ions are shown [27]. The transition wavelengths shown: 397 nm corresponds to the cooling transition (from the inital ground state of the ions) and 866 nm corresponds to the repumper (excitation out of the "dark" D state).

be studied using densities achievable under high vacuum in many different types of neutral and ion traps. The neutral atom trap we use and study at the UCONN group is a sodium MOT. A MOT uses red-detuned light in order to cool down atoms to the order of $\sim 100\mu K$, specifically 250 μK in the case of our sodium MOT. These cooled atoms are simultaneously collected by adding a spatial dependence on the light force via a magnetic gradient in the trapping region. When aligned with specifically chosen polarizations of light, the atoms are pushed to the center of the trap to form a cold and relatively dense (10^9 atoms/cm^3) cloud of atoms. An advantage of using a MOT is that we get specific control and diagnosis on the quantum states of the sodium atoms inside the trap. This will be very helpful later when quantifying the reactions we will be studying, since the reactions are differentiated by quantum state. These traps typcally have depths of $\sim$1 K or $\sim 10^{-4}$eV.

In order to measure these reactions however, we also need to trap ions in the same space as our atoms. The most common way this is done is with an r.f. Paul Trap. A Paul Trap operates using r.f. because of Earnshaw's theorem, which states generally that a collection of point charges cannot be trapped (in a stable equilibrium) with electrostatic forces. In other words, one must use an oscillating field in order to trap a charged particle from the field alone in more than one dimension. A Paul Trap does exactly this, using alternating r.f. on 4 rods, creating a saddle potential in two radial dimensions (x and y in Fig. 1). We oscillate the voltages out of phase with one another, which oscillates this saddle potential, creating what is referred to as a pseudopotential (time-averaged) conservative potential well in the radial direction. A voltage is applied to the end-caps in the other dimension, giving us total confinement for the ions. The UCONN trap has a depth of $\sim$1000 K, which enables us to study a range of collision energies up to $\sim$ .1 eV (center-of-mass) in our system.

2.2 Recent Work

There has been recent work done in our hybrid trap, namely an experimental determination of the total collision rate of Na and Na^+ [28]. Along with this, our group has studied the loading/steady state behavior of the hybrid trap [29] which shows complex effects. There has also been work relevant to the upcoming experiments. Namely, we devised and tested a locking arrangement for the lasers required for calcium ion cooling [30]. The lasers in this paper are 396.847 nm and 866.216 nm respectively used for the cooling and repumping of calcium ions [27]. The laser frequency schematic is depicted in Fig. 2. Our locking system yielded long-term stability of our commercial 397 nm laser of $2\pi \times 6.7(2)$ MHz and the custom-built 866 nm laser of $2\pi \times 8.6(2)$MHz. Compared to the natural linewidth of the 4p excited (Ca^+) state of $2\pi \times (20.7 + 1.7)$ MHz, our lasers are adequate for our experimental application to laser cool Ca^+.

2.3 Charge Exchange Mechanisms

For my thesis research, I plan to continue our group's study of charge-exchange collisions between Na and Ca^+. In 2014, our group published preliminary findings of our evidence for charge exchange, as well as the theoretical reaction rates in our hybrid trap [31]. It was found that under the presence of neutral sodium atoms in the MOT, Ca^+ ions were lost from the LPT as shown in Fig. 3 (left). Since the ion trap depth is quite large (~ 1 eV or 10^4 K), this loss mechanism introduced by the overlapping MOT was clearly not due to elastic scattering since the atoms in the MOT are much colder and slower (~ 100 μK) . Instead, it was hypothesized that the Ca^+ ions were lost from the trap by charge exchange collisions between the Na and Ca^+.

Studying Born-Oppenheimer molecular Potential Energy Curves (PECs) for the colliding ion-atom system can give us an idea of how charge-exchange collisions will happen. Each PEC is derived adiabatically, and so they can give a first order approximation to the molecular behavior during a collision. An avoided crossing between two PECs occurs when the two states in question have the same molecular symmetry; this is called the Wigner non-crossing rule. Since electronic transition timescales are much faster than the motion of the atom, there is a non-zero probability of the atom acting non-adiabatically and a transition occurring across an avoided crossing [32]. In the case where the electron is transferred between the atoms without any emission of a photon, we call this direct charge transfer. In the case where the transition to another potential curve is accompanied by the emission of a photon, the transition is called radiative charge transfer. Generally with direct charge transfer, a smaller gap between the two states results in a larger probability of a diabatic transition between the two molecular states that cross. Charge-transfer collisions can occur between quasi-molecular terms with different symmetry due to the Coriolis (rotational) interaction. If we
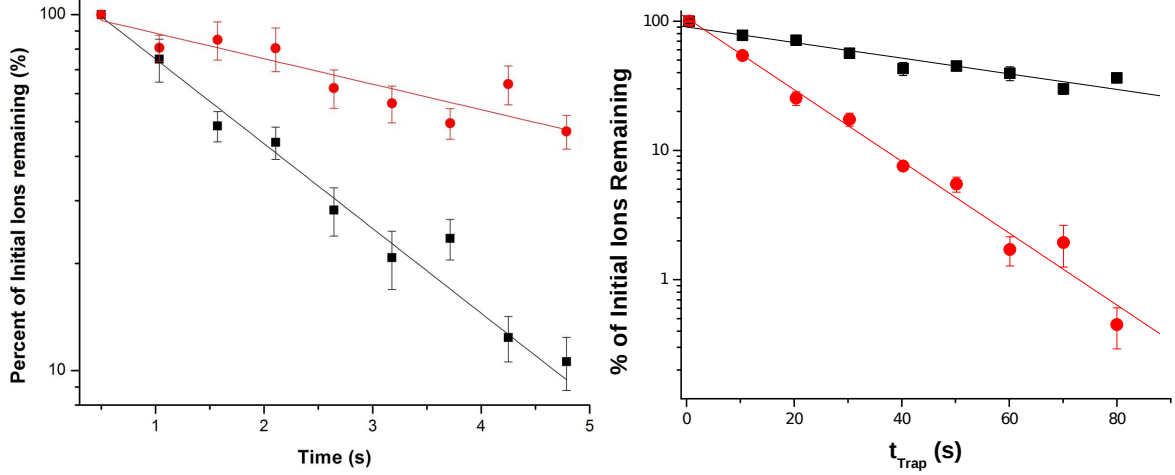
Figure 3: A log plot of the decay curves of the Ca^+ population (left) and the Na^+ population (right) in the hybrid trap. In each, the black square curve represents the addition of a MOT. Note that on the left, the Ca^+ ions decay faster with a colocated MOT while on the right, the Na^+ ions decay slower with the addition of the MOT. Error bars shown are calculated as standard error of multiple measurements.

analyze our given PECs for Na and Ca, we can determine qualitatively which of these transitions are most probable. In reality, the cross-sections are typically calculated by theoretical physicists or quantum chemists, which we will compare to.

From the initial calculations of the PECs, there are three singlet Σ molecular states which would warrant study as possible entrance channels for a charge exchange collision (See Fig. 4):

(i) $5^1\Sigma^+ \rightarrow 4^1\Sigma^+, X^1\Sigma^+$:

The first candidate for charge exchange is the highest energy (currently attainable) PEC, the entrance channel $Na[^2P] + Ca^+[^2S]$. The molecule in the 5th singlet Σ state can either undergo direct charge transfer into the 4 singlet state or radiative charge transfer into the ground state, where it is possible to form a molecule. In this entrance channel, there is a potential barrier of ~ 0.017 eV or ~ 200K in Fig. 4 which warrants study. Since the sodium atoms are in a MOT, they are already cold ($\sim 250 \mu$K), so we can laser cool the Ca^+ to get both reactants below this potential barrier. If we cool below the potential barrier, this will "shut off" both of these reaction pathways, and should give us an idea as to whether or not it was a significant contributor to our observed total charge-exchange rate. Through preliminary results, there is already some evidence of this reaction shutting off, which could be the result of the hot ions in the trap reacting with the sodium and leaving only a cold plasma/Coulomb crystal of Ca^+.

(ii) $3^1\Sigma^+ \rightarrow 2^1\Sigma^+$:

The second relevant candidate for charge exchange is the entrance channel $Na[^2S] + Ca^+[^2D]$. This is
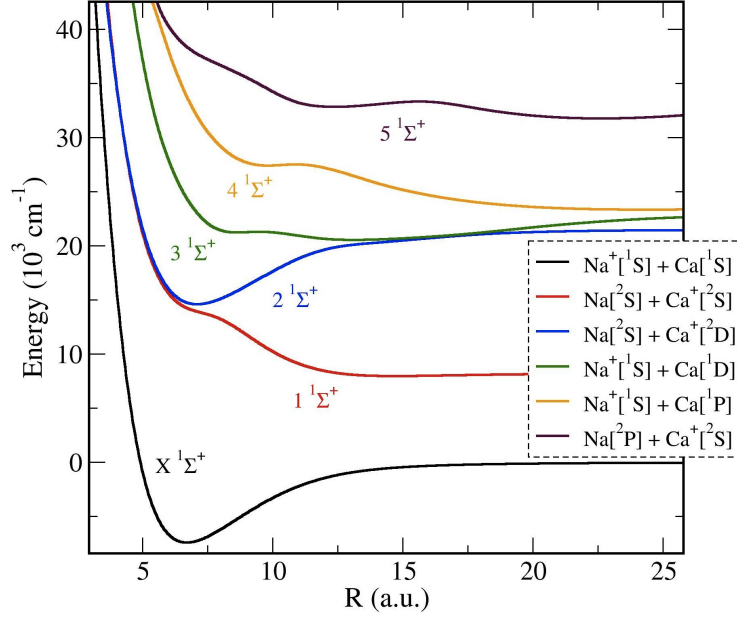
6

Figure 4: The singlet Σ state PECs are shown for the first 6 lowest molecular states. Interesting features include a barrier in the $5^1\Sigma^+$ state, which would prevent a reaction. Similar updated curves are being calculated for the singlet Σ and triplet Σ and Π states by Brendan MacLaughlin[34]. The atomic/ionic asymptotes are listed in the box in increasing order of energy. (courtesy of Sandipan Banerjee and Harvey Michels, private communication 2012)

only a viable entrance channel if the metastable D state (see Fig. 2) is populated. Since the ionized calcium in the previous experiment was most likely not excited to this D state, this was likely not the loss mechanism observed in prior experiments. However, we can still populate this state and test how that affects the reaction rate in the hybrid trap (see proposed research).

(iii) $1^1\Sigma^+ \rightarrow X^1\Sigma^+$:

Another possible candidate for charge exchange worth mentioning is the ground state entrance channel, $Na[^2S] + Ca^+[^2S]$. Calculations were done that showed this rate is exceedingly small, and not worth looking into as a potential contribution to our total scattering rate. In support of this conclusion, we found that our preliminary rate goes to zero (non-measurable) as $f_e \rightarrow 0$, which would imply that the rate measured has no contribution from the ground state Na. Since we can trap Ca^+ for ~ 15 minutes or more, we might be able to see some of this reaction [33].

Because of the limits of our experiment, these are all of the initial singlet states we can efficiently prepare in sufficient density and consistency to make any meaningful measurements of rate. While there are triplet curves that warrant study, they will not be addressed here, as the principles are similar and the rates of the states of interest have not all been calculated yet [34]. There are also no barriers in the triplet molecular

curves, which would lead us to believe that the rate we have observed with our preliminary data does not have any significant contributions from the triplet states and is dominated by our first proposed process, (i).

2.4   Excited State Fraction

In order to make rate measurements which differentiate between the ground and excited sodium targets, we must understand the total atom distribution in ground and excited state hyperfine levels. Typically f_e is not directly measured, but instead modeled with an idealized two-level model based on the steady state solution to the optical Bloch equations

$$f_e = \left(\frac{1}{2}\right) \frac{I/I_{sat}}{1 + I/I_{sat} + (2\delta/\Gamma)^2},\tag{1}$$

where I is the total MOT laser intensity, δ is the detuning from atomic resonance, and Γ is the transition's linewidth [35, 4]. In this equation, the saturation intensity I_{sat} is defined as

$$I_s = \frac{\hbar\omega^3\Gamma}{12\pi c^2},\tag{2}$$

where ω is the angular frequency of the MOT laser beams, and $\hbar$ and c are fundamental constants. However, this predicted value for I_{sat} is almost never appropriate in the real world, since the atoms we work with are not strictly two-level. An example of this is when a similar measurement was performed on rubidium using recoil spectroscopy [5, 6]. In their study, they found that f_e followed the two-level model with an adjusted I_{sat} up to around $2I_{sat}$. In our case, we can make MOTs on two different transitions with sodium. The Type I MOT is pumped from $F = 2 \rightarrow F' = 3$, while the Type II MOT uses the cycling transition from $F = 1 \rightarrow F' = 0$ (This is shown in Fig. 1). For the Type I MOT, the closest state to the cycling transition (or "repump state") is the $F' = 2$, which is ~ 58 MHz detuned. Conversely for the Type II MOT, the $F' = 1$ repump state is ~ 16 MHz detuned from the main transition [35]. These spacings are small compared to the rubidium excited state spacing of ~ 266 MHz, which implies that any non-two-level effects will be more apparent in our two sodium MOTs. Since the rubidium MOT already demonstrates that the f_e behavior deviates from the model at a relatively small intensity (relative to I_{sat}), we expect that the sodium MOT will deviate further from the model and present some state-mixing effects as well. This means that in order to obtain an accurate measurement of any reaction rates with the MOT as the target, we must measure f_e directly.

3 Proposed Research

The following experiments were chosen because they investigate interesting phenomena in a hybrid trap. The results of these experiments will give publication-worthy results, and have a positive impact on the field of hybrid traps and cold quantum chemistry.

3.1 Excited State Fraction Direct Measurement (Model Independent)

First we propose to directly measure the excited state fraction of our sodium MOT. More specifically, the excited state fraction of a sodium MOT is the number of atoms in the $^3P_{3/2}$ state. Since the sodium hyperfine level structure is much more closely spaced than previously studied systems, the sodium MOT should deviate further from the expected two-level model used to predict the excited state fraction. Based on our preliminary results, there are additional strong deviations from the model that may be due to state-mixing in a sodium MOT, a result of power broadening into a secondary state (3 or more level model), as well as Autler-Townes. This means that the model deviation will depend on things like detuning, magnetic gradient, and repump power. This additional deviation from the model will be worth study for anyone who needs a precise measurement of f_e in a MOT made of an atom with a narrow upper hyperfine manifold. In order to perform a direct measurement, we independently calculate loss rates from the MOT due to excited state photoionization (PI) via fluorescence measurements and ionization measurements. First, we use the photomultiplier tube to measure the MOT loading rate via fluorescence with and without PI. Then, we utilize the hybrid trap to trap the ions and determine a separate photoionization rate from the number of the extracted ions. We will need to calibrate the channeltron signal to determine how many ions were created from the photoionization of the MOT. This can be done using existing lasers and crystallization techniques, by imaging and counting calcium ions in the trap and extracting to determine a ratio between detection signal and ion number. Here we assume that the collection efficiency of the detection scheme is the same for both calcium and sodium ions.

3.2 Charge Exchange

Once we have properly quantified f_e of the sodium MOT, we will be able to measure the total number of atoms in the trap via fluorescence measurements. Additionally, accurately knowing f_e and the total number will enable us to count the number of atoms in each quantum state, which is necessary to accurately measure reaction rates. We can use this characterized MOT to then probe the previously discussed reaction channels between sodium and ionized calcium.

We will begin the study of charge exchange by looking at the interactions between the MOT and ground

state ionized calcium. The reactants in this case can take two pathways to charge exchange, the first through direct charge transfer ($5^1\Sigma^+ \rightarrow 4^1\Sigma^+$) and the second through radiative charge transfer ($5^1\Sigma^+ \rightarrow X^1\Sigma^+ + h\nu$). Radiative charge-transfer is much less likely than direct charge-transfer. Calculations are underway to determine the expected ratio of these two processes. During this reaction, we apply an AC voltage to the LPT known as mass-selective resonance quenching (MSRQ) at the trap's secular frequency for a particular ion mass [36]. Using MSRQ allows us to exclude ions from the trap based on mass. This is how we are able to detect the charge transfer: We start with Ca^+ ions in the LPT, and apply MSRQ to exclude anything with the mass of sodium. When charge transfer occurs, the calcium is no longer trapped, and the Na^+ is ejected from the trap. This can be detected as a fractional loss of Ca^+ ion population from the initial ion population. While this method does not allow us to distinguish between the two channels, there is a possibility of molecular formation in the $X^1\Sigma^+$ ground state. If this reaction occurs and we create molecular $(NaCa)^+$, we would be able to distinguish them from free sodium ions using MSRQ. The ratio between molecular formation and separated atoms can be calculated and compared to experiment.

In preliminary results, we have observed that the reaction between excited 3p Na MOT atoms and ground state ionized calcium shuts off when the collision energy is below the barrier. We hypothesize that this is due to the hot calcium ions reacting, leaving only the cold ions which are below the collisional energy required to react. Previous results reported in this proposal show all of the ions reacting, which would be consistent with this hypothesis since that experiment was done with a hotter initial sample of ions. With our LPT, we have the ability to heat up our ions through excess micromotion (occurs as the ions are trapped off of the center axis). Our hypothesis of a temperature barrier can be tested by heating up our ions, and determining if the reaction affects a larger portion/all of the ions. Additionally, we have lasers that can be used to cool the calcium ions, much like the lasers in the MOT. We could further test the barrier theory by crystallizing the calcium ions, which would bring them to ~ 1 mK, well below the .017 eV barrier. This, if effective, would further support the existence of the barrier, and the notion that our total rate measurement from the initial states prepared is dominated by contributions from the excited sodium in the $5^1\Sigma^+$ state. In addition to this, we can populate the $^2P_{1/2}$ state by using both the cooling and repump lasers for Ca^+, and the $^2D_{3/2}$ state by turning off the repumper, which could lead to more interesting and valuable comparisons to the theoretically calculated rates for other specific reaction channels.

4   Conclusion

Here we have detailed two experiments that would allow for the analysis of ion-neutral interactions in a hybrid trap containing Na and Ca^+. Ion-neutral interactions have very large, measurable cross sections and

reaction rates compared to neutral-neutral collisions. Using the hybrid trap, we can exploit these large cross sections and rates to compare with theoretically calculated rates of our system as they become available[34]. Additionally, we have detailed how we can perform a novel, direct measurement of the excited state fraction of a sodium MOT, which will enable us to obtain much more accurate measurements of our ion-neutral reaction rates. This work will be done under the supervision of Prof. Winthrop Smith in collaboration with previous group members Prof. Douglas Goodman and Prof. James Wells, as well as Dr. Francesco Narducci and Prof. Reinhold Blümel of Wesleyan University.

References

[1] R. Côté and A. Dalgarno. Ultracold atom-ion collisions. *Phys. Rev. A.*, 62(1):012709.

[2] Eric R. Hudson. Method for producing ultracold molecular ions. *Phys. Rev. A.*, 79(3):032716.

[3] Winthrop W. Smith, E. Babenko, R. Côté, and Harvey H. Michels. On the collisional cooling of co-trapped atomic and molecular ions by ultracold atoms: $Ca^+ + Na$ and $Na_2^+(v^*, J^*) + Na$. In N. P. Bigelow, J. H. Eberly, C. R. Stroud Jr, and I. A. Walmsley, editors, *Coherence and Quantum Optics VIII (No.8)*, pages 623–624. Kluwer Academic/Plenum.

[4] E. L. Raab, M. Prentiss, Alex Cable, Steven Chu, and D. E. Pritchard. Trapping of neutral sodium atoms with radiation pressure. *Phys. Rev. Lett.*,59(23):2631–2634.

[5] M. H. Shah, H. A. Camp, M. L. Trachy, G. Veshapidze, M. A. Gearba, and B. D. DePaola. Model-independent measurement of the excited fraction in a magneto-optical trap. *Phys. Rev. A*, 75(5):053418, May 2007.

[6] G. Veshapidze, J.-Y. Bang, C. W. Fehrenbach, H. Nguyen, and B. D. DePaola. Model-free measurement of the excited-state fraction in a ^{85}Rb magneto-optical trap. *Phys. Rev. A*, 91:053423, May 2015.

[7] W. Neuhauser, M. Hohenstatt, P. E. Toschek, and H. Dehmelt. Localized visible Ba^+ mono-ion oscillator. *Phys. Rev. A*, 22(3):1137–1140.

[8] M.G. Raizen, J.M. Gilligan, J.C. Bergquist, W.M. Itano, and D.J. Wineland. Linear trap for high-accuracy spectroscopy of stored ions. *J. Mod. Opt.*, 39(2):233–242.

[9] R. Blatt, P. Gill, and R. C. Thompson. Current perspectives on the physics of trapped ions. *J. Mod. Opt.*, 39(2):193–220.

[10] J. D. Prestage, G. J. Dick, and L. Maleki. New ion trap for frequency standard applications. *J. App. Phys.*, 66(3):1013–1017.

[11] S. A. Diddams, Th. Udem, J. C. Bergquist, E. A. Curtis, R. E. Drullinger, L. Hollberg, W. M. Itano, W. D. Lee, C. W. Oates, K. R. Vogel, and D. J. Wineland. An optical clock based on a single trapped ^{199}Hg$^+$ ion. *Science*, 293(5531):825–828.

[12] D. Leibfried, E. Knill, S. Seidelin, J. Britton, R. B. Blakestad, J. Chiaverini, D. B. Hume, W. M. Itano, J. D. Jost, C. Langer, R. Ozeri, R. Reichle, and D. J. Wineland. Creation of a six-atom 'Schrödinger cat' state. *Nature*, 438(7068):639–642.

[13] J. I. Cirac and P. Zoller. Quantum computations with cold trapped ions. *Nature*, 74(20):4091–4094.

[14] Kilian Singer, Ulrich Poschinger, Michael Murphy, Peter Ivanov, Frank Ziesel, Tommaso Calarco, and Ferdinand Schmidt-Kaler. *Colloquium* : Trapped ions as quantum bits: Essential numerical tools. *Rev. Mod. Phys.*, 82(3):2609–2632.

[15] Andrew T. Grier, Marko Cetina, Fedja Oručević, and Vladan Vuletić. Observation of cold collisions between trapped ions and trapped atoms. *Phys. Rev. Lett.*, 102(22):223201.

[16] Wade G. Rellergert, Scott T. Sullivan, Svetlana Kotochigova, Alexander Petrov, Kuang Chen, Steven J. Schowalter, and Eric R. Hudson. Measurement of a large chemical reaction rate between ultracold closed-shell ^{40}Ca atoms and open-shell ^{174}Yb$^+$ ions held in a hybrid atom-ion trap. *Phys. Rev. A*, 107(24):243201.

[17] Scott T. Sullivan, Wade G. Rellergert, Svetlana Kotochigova, Kuang Chen, Steven J. Schowalter, and Eric R. Hudson. Trapping molecular ions formed via photo-associative ionization of ultracold atoms. *Phys. Rev. A*, 13(42):18859.

[18] Scott T Sullivan, Wade G Rellergert, Svetlana Kotochigova, and Eric R Hudson. Role of Electronic Excitations in Ground-State-Forbidden Inelastic Collisions Between Ultracold Atoms and Ions *Phys. Rev. Lett.*, 109(22): 223002.

[19] Christoph Zipkes, Stefan Palzer, Carlo Sias, and Michael Köhl. A trapped single ion inside a Bose-Einstein condensate. *Phys Rev. Lett.*, 464:388–391.

[20] Christoph Zipkes, Stefan Palzer, Lothar Ratschbacher, Carlo Sias, and Michael Köhl. Cold heteronuclear atom-ion collisions. *Phys. Rev. Lett.*, 105(13):133201.

[21] Lothar Ratschbacher, Christoph Zipkes, Carlo Sias, and Michael Köhl. Controlling chemical reactions of a single particle. *Nature Physics*, 8(9):649–652.

[22] L. Ratschbacher, C. Sias, L. Carcagni, J. M. Silver, C. Zipkes, and M. Köhl. Decoherence of a single-ion qubit immersed in a spin-polarized atomic bath. *Phys. Rev. Lett.*, 110(16):160402.

[23] Stefan Schmid, Arne Härter, and Johannes Hecker Denschlag. Dynamics of a cold trapped ion in a Bose-Einstein condensate. *Phys. Rev. Lett.*, 105(13):133202.

[24] A. Härter and J. Hecker Denschlag. Cold atomion experiments in hybrid traps. *Contemporary Physics*, 55(1):33–45.

[25] Shinsuke Haze, Sousuke Hata, Munekazu Fujinaga, and Takashi Mukaiyama. Observation of elastic collisions between lithium atoms and calcium ions. *Phys. Rev. Lett.*, 87(5):052715.

[26] Winthrop W. Smith, Oleg P. Makarov, and Jian Lin. Cold ion-neutral collisions in a hybrid trap. *J. Mod. Opt.*, 52(16):2253–2260.

[27] Alexander D. Gingell, Martin T. Bell, James M. Oldham, Timothy P. Softley, and Jeremy N. Harvey. Cold chemistry with electronically excited Ca$^+$ coulomb crystals. *J. Chem. Phys.*, 133, 194302.

[28] D. S. Goodman, J. E. Wells, J. M. Kwolek, R. Blümel, F. A. Narducci, and W. W. Smith. Measurement of the low-energy Na$-$Na$^+$ total collision rate in an ion-neutral hybrid trap. *Phys. Rev. A*, 91(1):012709.

[29] R. Blümel, J. E. Wells, D. S. Goodman, J. M. Kwolek, and W. W. Smith. Universal nonmonotonic structure in the saturation curves of magneto-optical-trap-loaded Na$^+$ ions stored in an ion-neutral hybrid trap: Prediction and observation. *Phys. Rev. A*, 92(6):063402.

[30] J. M. Kwolek, J. E. Wells, D. S. Goodman, and W. W. Smith. Simple locking of infrared and ultraviolet diode lasers to a visible laser using a LabVIEW proportional-integral-derivative controller on a fabry-perot signal. *Review of Scientific Instruments*, 87(5):055102.

[31] W. W. Smith, D. S. Goodman, I. Sivarajah, J. E. Wells, S. Banerjee, R. Côté, H. H. Michels, J. A. Mongtomery Jr., and F. A. Narducci. Experiments with an ion-neutral hybrid trap: cold charge-exchange collisions. *Appl. Phys. B: Lasers and Optics*, 114(1):75–80.

[32] William C. Stwalley, Michael Bellos, Ryan Carollo, Jayita Banerjee, and Matthew Bermudez. Shortcuts for understanding rovibronic spectroscopy of ultracold alkali metal diatomic molecules. *Molecular Physics*, 110(15):1739–1755.

[33] Oleg P. Makarov, R. Côté, and W. W. Smith. Radiative charge-transfer lifetime of the excited state of $(NaCa)^+$. *Phys. Rev. A*, 67, 042705.

[34] B. McLaughlin and J. Babb. Calculations in progress. *Private Communications*, (2017).

[35] Daniel Adam Steck. *Sodium D Line Data*. Jan 2010. Available online at http://steck.us/alkalidata (revision 2.1.4, 23 December 2010).

[36] Takashi Baba and Izumi Waki. Cooling and mass-analysis of molecules using laser- cooled atoms. *Japanese Journal of Applied Physics*, 35(Part 2, No. 9A):L1134 L1137, 1996.