

## Research Article

# Moment Theories of Ion Motion and Ion-Neutral Reactions in Linear Traps

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**Abstract.** Moment theories of ion motion and reaction in ideal and stretched quadrupole ion traps are extended to the case of linear ion traps. Fortran and Mathematica computer programs based on these theories are developed. They are applied to the case of  $O^+$  ions moving through an Ar buffer gas containing a small amount of a reactive neutral,  $N_2$ . The rate coefficient predicted *ab initio* for a common set of trap parameters is  $6.4 \pm 0.9 \times 10^{-13} \text{ cm}^3/\text{s}$ , which is large enough that it should be measurable.

**Keywords:** ion traps, linear trap, quadrupole trap, gaseous ion transport, numerical simulation

## 1. Introduction

Starting from the Boltzmann equation, two-temperature (2T) and multitemperature (MT) moment theories for the motion of trace amounts of ions in devices where there are external fields that vary with position and time were presented in the first [1] of a series of papers. The accuracy of the 2T theory was demonstrated in the second paper [2], which considered field-asymmetric ion mobility spectrometry (also called differential mobility spectrometry). The 2T theory was applied in the third paper [3] to ideal quadrupole ion traps (sometimes called 3D quadrupole ion traps), where it was shown to be more directly connected to other theories [4] than is the MT theory, even though the MT theory is expected to be more accurate. The final papers of the series

[5, 6] extended the theories of the first paper to encompass stretched quadrupole traps containing molecular ions and neutrals, with the use of spherical-polar basis functions (the SB theory) corresponding to the 2T theory for atomic systems and the use of Cartesian basis functions (the CB theory) corresponding to the MT theory.

In subsequent papers [7, 8], we extended these theories to situations in which a small fraction of the neutral gas is a species that can undergo infrequent reaction with the ion of interest. We found that, in the first of a series of successive approximations, the measured ion-neutral reaction rate coefficients employing time- and space-dependent electric fields can be equated to thermal rate coefficients appropriate to high temperatures in the absence of an electric field. This is the case even though the velocity distribution function of the ions

may differ substantially from an equilibrium distribution. Further, we provided differential equations for the position- and time-dependent moments of ion velocity and energy that are necessary to convert the actual experimental parameters into the corresponding elevated temperature.

The papers just summarized were generalized beyond ion traps into uniform moment theories for charged particle motion in gases [9]. The first approximation of the uniform theory when applied to ion traps reproduces the first approximation results of the other papers. Moreover, consideration of the second approximation of the uniform 2T theory for drift-tube mass spectrometers shows (in work to be published) that the successive approximations are converging. The purpose of the present paper is to apply the uniform moment theories to linear ion traps (sometimes called 2D ion traps), which are now more commonly used than ideal or stretched quadrupole ion traps. Because we are assuming that only trace amounts of ions are present, space-charge effects are not considered in the previous papers or in this one.

We begin by presenting the general differential equations governing the average ion velocity and energy that arise in the first approximation of the various moment theories. The electric fields are given in the next section for quadrupole and linear ion traps. The specific first-approximation moment equations in both types of ion trap are then given. Tests of two computer programs based on the equations in the previous section are given for the special cases where the ion-neutral collisions follow the Maxwell model of constant collision frequency and the rigid-sphere model of constant cross section. Also considered is the reaction rate coefficient for  $^{107}\text{Ag}^+$  ions reacting with  $\text{D}_2$  that is immersed in a much larger amount of He in a quadrupole ion trap; it is based on an *ab initio* interaction potential for  $\text{Ag}^+$  with He. We then consider the *ab initio* rate coefficient for the reaction of  $^{16}\text{O}^+$  ions with  $\text{N}_2$  that could be measured in a linear trap containing argon buffer gas at 300 K. Finally, the results are summarized and discussed.

## 2. First-Approximation Moment Equations

Since there are no magnetic fields in radiofrequency ion traps, it can be shown that each of the four moment theories leads in first approximation to an ordinary differential equation of the same form [6, 9]:

$$\frac{d}{dt}\bar{v}_u - \frac{q}{m}\mathbf{E}_u + \xi_u\bar{v}_u = 0. \quad (1)$$

This equation governs the time,  $t$ , evolution of the component of the average ion velocity,  $\bar{v}_u$ , along the Cartesian axis  $u$ , with  $u = x, y, z$ . Here  $\mathbf{E}_u$  is the component along  $u$  of the external electric field,  $q$  and  $m$  are the ion charge and mass, and  $\xi_u$  is the collision frequency for momentum transfer along direction  $u$ . As discussed in Appendix A, the microscopic definition of  $\xi_u$  depends upon which theory is used. Finally, each of the subscripted quantities in equation

(1) can depend upon position,  $\mathbf{r}$ , and time,  $t$ , but for simplicity this dependence is not explicitly indicated.

As pointed out previously [1], the moment equation (1) is equivalent to the damped Mathieu equation so often used to study ion motion in traps. The Mathieu equation is obtained from Newton's equation of motion for a single ion by assuming that the forces involved in that equation are external electrical forces and by adding in a damping term (with a constant collision frequency,  $\xi_u$ ) to mimic the effect of the forces that arise due to collisions. Equation (1), however, is obtained from the Boltzmann equation (in the first of a series of successive approximations) in which both external fields and ion-neutral interactions are treated correctly. It governs the average velocity of a group of ions in a trap at the same time, rather than the motion of a single ion.

The various expressions for  $\xi_u$  depend upon the gas temperature,  $T$ , and one or more effective ion temperatures that can be considerably larger than  $T$  because the ions are present only in trace amounts in the apparatus. Therefore, equation (1) must be coupled to differential equations governing these ion temperatures. In the first approximation of the 2T and SB theories,  $\xi_u$  is independent of the direction, so the subscript can be dropped. More importantly, it is a function only of the effective temperature,  $T_{\text{eff}}$ , that is governed by the equation [6, 9]:

$$\begin{aligned} & \frac{d}{dt} \left[ \frac{3}{2} k_B T_{\text{eff}} \right] \\ & - \frac{q\mu}{m} \mathbf{E} \cdot \bar{\mathbf{v}} + \frac{2\mu\xi}{M} \left[ \frac{3}{2} k_B (T_{\text{eff}} - T) + \frac{M\Phi}{m} \left( \frac{3}{2} k_B T_{\text{eff}} \right) \right] = 0. \end{aligned} \quad (2)$$

Here  $\mu$  is the ion-neutral reduced mass,  $k_B$  is Boltzmann's constant,  $M$  is the neutral mass, and  $\Phi$  is the dimensionless ratio of the collision integral for inelastic energy loss to that for momentum transfer that is discussed in Appendix B. It should be noted that the collision frequency couples each  $\bar{v}_u$  to  $T_{\text{eff}}$  and hence that all of the  $\bar{v}_u$  are coupled. Finally,  $\Phi = 0$  for atomic ion-neutral systems, where the SB theory reduces to the 2T theory.

In first approximation of the MT and CB theories, the collision frequencies depend on ion temperatures,  $T_{u,\text{eff}}$ , that may differ along the various Cartesian axes. These effective temperatures are governed by the following equation [6, 9]:

$$\begin{aligned} & \frac{d}{dt} \left[ \frac{1}{2} k_B T_{u,\text{eff}} \right] \\ & - \frac{q\mu}{m} \mathbf{E}_u \bar{v}_u \\ & + \frac{2\mu\xi_u}{M} \left[ \frac{1}{2} k_B (T_{u,\text{eff}} - T) + \frac{M\Phi_u}{m} \left( \frac{1}{2} k_B T_{u,\text{eff}} \right) \right] = 0. \end{aligned} \quad (3)$$

There are three differential equations represented by equation (3), as opposed to one represented by equation (2). In addition, the dimensionless ratios  $\Phi_u$  in equation (3) provide for energy partitioning as well as inelastic energy transfer,

as discussed in Appendix B. The  $\Phi_u$  are all zero for atomic ion-neutral systems, where the CB theory reduces to the MT theory.

The collision frequencies in the SB and CB theories depend not only upon the effective temperature above but also upon an internal ion temperature that is equivalent to the average internal energy of the molecular ions. In both theories, the differential equation governing  $T_{int}$  has the same form, which is given in [6] and so needs not be repeated here.

The ion number density,  $n$ , at all positions in the apparatus and at all times can be obtained by solving the rate equation of continuity:

$$\frac{\partial}{\partial t} n + \nabla \cdot n\bar{v} = -kn, \quad (4)$$

where  $k$  is the second-order reaction rate coefficient. This equation can be solved by a forward-time, forward-space version of the finite difference method [10], provided that we have knowledge of the ion number density (as a function of position) at time  $t = 0$ . Here, as in previous work [8], we assume that the initial ion number density is normally distributed along each Cartesian axis, with standard deviations  $\sigma_x$ ,  $\sigma_y$ , and  $\sigma_z$  that may be different. This choice has the advantage that it should apply when no special experimental techniques have been implemented. In order to match results in a particular experiment, however, it may be necessary to work with other initial ion number density functions.

For the two-temperature theory for atomic ions moving in a background gas of atomic neutrals and reaction with a trace amount of a single reactive neutral (whether atomic or molecular), the reaction rate coefficient is given by the following equation [7, 9]:

$$k(t) = \left( \frac{8k_B T_{R,\text{eff}}}{\pi\mu_R} \right)^{1/2} \int_0^\infty \exp(-\gamma^2) Q_R^*(\gamma^2 k_B T_{R,\text{eff}}) \gamma^3 d\gamma, \quad (5)$$

where  $\mu_R$  is the reduced mass for the ion and reactive neutral with mass  $M_R$ . In addition,

$$T_{R,\text{eff}} = \frac{mT}{m + M_R} \left( 1 - \frac{M_R}{M} \right) + \frac{M_R(m + M)}{M(m + M_R)} T_{\text{eff}}, \quad (6)$$

and  $Q_R^*$  is the total reactive cross sections, that is, a function of the reactive collision energy,  $\gamma^2 k_B T_{R,\text{eff}}$ . Since  $T_{\text{eff}}$  depends upon position and time, so does both  $T_{R,\text{eff}}$  and  $k(t)$ . Equation (5) must be integrated over all spatial positions in order to determine the rate coefficients for all ions in the trap at a particular time:

$$\bar{k}(t) = \frac{1}{n_0} \iiint_{-\infty}^{\infty} n(x, y, z, t) k(x, y, z, t) dx dy dz. \quad (7)$$

This result must, in turn, be integrated over many cycles of the ac fields that are present or equivalently over one cycle at

large enough times that steady-state behavior occurs, in order to obtain the single value,  $k$ , that applies to the trap as a whole when no changes in external parameters are imposed.

For the MT theory in similar systems, we have

$$k(t) = \frac{1}{2\pi} \left( \frac{2k_B T}{\pi\mu_R} \right)^{1/2} \times \iiint_0^\infty \exp(-\gamma_x^2 - \gamma_y^2 - \gamma_z^2) Q_R^*(\epsilon_R^*) \left( \frac{\epsilon_R^*}{k_B T} \right)^{1/2} d\gamma_x d\gamma_y d\gamma_z, \quad (8)$$

where

$$\epsilon_R^* = \gamma_x^2 k_B T_{R,x,\text{eff}} + \gamma_y^2 k_B T_{R,y,\text{eff}} + \gamma_z^2 k_B T_{R,z,\text{eff}}. \quad (9)$$

The effective temperatures in equation (9) are related to the  $T_{u,\text{eff}}$  in the same way that  $T_{R,\text{eff}}$  is related to  $T_{\text{eff}}$ , that is, by equation (6). The MT expression given here differs by a factor of 2 from that given previously [7], so that it reduces to equation (5) in the limit where the three effective temperatures are all the same.

It should be noted that  $Q^*$  must be computed for molecules by adding state-specific cross sections, weighted so as to take into account the probability of having that particular state present. Since we will not apply the present work to situations where either the ion or the buffer gas is molecular, no further comments about the treatment of reactions in the SB and CB theories are necessary, other than to note that the reactive neutrals can be molecular when the 2T or MT theories are used.

### 3. Electric Fields in Traps

In an ideal quadrupole ion trap, the hyperbolic endcap electrodes are fixed at ground potential and a time-dependent voltage,  $U + V \cos(\Omega_{RF}t)$ , is applied to the ring electrode. Here  $U$  is the amplitude of the dc voltage and  $V$  is the zero-to-peak amplitude of the ac component that has angular frequency  $\Omega_{RF}$ . The resulting electric field is purely linear; in that at a particular point in the apparatus it has components that are directly proportional to the position. The standard way [3] of expressing the field is

$$E_u = -\frac{m\Omega_{RF}^2}{4q} [a_u - 2q_u \cos(\Omega_{RF}t)] u, \quad (10)$$

where

$$a_z = -2a_x = -2a_y = \frac{-16qU}{m(r_0^2 + 2z_0^2)\Omega_{RF}^2} \quad (11)$$

and

$$q_z = -2q_x = -2q_y = \frac{8qV}{m(r_0^2 + 2z_0^2)\Omega_{RF}^2}. \quad (12)$$

Here it is assumed that the origin of the coordinate system is at the center of the ring electrode with internal radius  $r_0$  and that  $2z_0$  is the shortest distance between the endcap electrodes.

The fields are more complicated in a stretched or otherwise nonideal quadrupole trap, even though it is cylindrically symmetric along the  $z$  axis. The endcap electrodes are identical and arranged symmetrically, with a time-dependent voltage applied between them in a dipolar fashion, so that one has  $[U_D + V_D \cos(\omega_D t + \delta_D)]/2$  while the other has a negative value of exactly the same magnitude. Here  $U_D$ ,  $V_D$ , and  $\omega_D$  are the equivalents of  $U$ ,  $V$ , and  $\Omega_{RF}$ . Note the phase shift,  $\delta_D$ , that may be present between this potential and that applied to the ring electrode. Then the total electric potential can be expressed [11] as a multipole expansion. The resulting electric field can be written as [4]

$$E_u = -\frac{m\Omega_{RF}^2}{4q} \left( [\tilde{a}_u - 2\tilde{q}_u \cos(\Omega_{RF}t)] u + [\tilde{b}_u - 2\tilde{d}_u \cos(\omega_D t + \delta_D)] \tilde{f}_u \right), \quad (13)$$

where the quantities marked with a tilde are given in Table 1 in terms of the quantities above and

$$b_z = -2b_x = -2b_y = \frac{-16qU_D}{m(r_0^2 + 2z_0^2)\Omega_{RF}^2}, \quad (14)$$

$$d_z = -2d_x = -2d_y = \frac{8qV_D}{m(r_0^2 + 2z_0^2)\Omega_{RF}^2}. \quad (15)$$

The signs in some of the entries in Table 1 correct errors in the previous paper [4]. The ellipses indicate higher-order multipole terms that are usually assumed to be zero based on the values for the coefficients,  $A_n$ , that are collected in [6] for several types of quadrupole traps.

Turning our attention now to linear traps, we note first that there are various geometries in use [12]. For example, there are linear traps with hyperbolic rods or slits in one pair of rods and others with a stretch in the electrode separation. We leave moment theories of such traps to later work and study here a simple geometry in which the linear ion trap has a total length of  $2z_0$  between flat endcaps and is made of four identical, parallel rods, symmetrically arranged, with each pair separated by a gap of distance  $2r_0$ . (Note that  $r_0$  and  $z_0$  have different meanings for linear traps than for quadrupole ion traps.) There has been some dispute [13] about the best radius,  $r$ , to use for the rods, but here we will use the relationship [14]  $r = 1.12590r_0$ .

In order to maintain as close a relationship as possible to the equations used for quadrupole ion traps, we will use equations (9)–(10) and (12)–(13) for linear traps, even though researchers in this area often choose definitions such that the  $x$  and  $y$  components in these equations have opposite signs from one another. As a further comment, we assume that the

user of the computer programs we discuss below will choose values of  $r_0$  and  $z_0$  so that any fringe fields due to the finite size of the electrodes are negligible.

The electrical potential due to a voltage of the form  $U + V \cos(\Omega_{RF}t)$  applied on two opposing rods, while the other two are held at ground, is independent of  $z$  and is given by the following equation [14]:

$$\begin{aligned} \phi_{rods}(x, y, t) &= [U + V \cos(\Omega_{RF}t)] \\ &\times \left[ A_2 \frac{x^2 - y^2}{r_0^2} + A_6 \frac{x^6 - 15x^4y^2 + 15x^2y^4 - y^6}{r_0^6} \right. \\ &+ A_{10} \frac{x^{10} - 45x^8y^2 + 210x^6y^4 - 210x^4y^6 + 45x^2y^8 - y^{10}}{r_0^{10}} \\ &\left. + \dots \right]. \end{aligned} \quad (16)$$

The numerical values for the constants in equation (16) are sensitive to the electrode size [15]. For the case  $r = 1.12590r_0$  that is used here, they are  $A_2 = 1.001462$ ,  $A_6 = 0.001292$ , and  $A_{10} = -0.002431$ , and we assume that all of the higher-order terms can be neglected. For another common situation [16, 17], where  $r = 1.14511r_0$ , the constants are slightly different [18, 19]. We also note that [20] sets all of the other coefficients above  $A_2$  to zero and incorporates  $A_2 = 1/2$  into the dimensionless parameters.

The more complicated linear ion traps mentioned above could require terms like  $A_4$  and  $A_8$ , but the straightforward addition of such terms to equation (16) is left to subsequent papers where such traps are considered. We also note that if an RF field is applied in a symmetric fashion, that is, with the same amplitude on all rods but 180 degrees out of phase for neighboring rods, then all that is involved is a modification of the constants in equation (16).

We assume that fringe fields due to the finite size of the ion trap are negligible. Then the electrical potential due to a voltage of the form  $U_D + V_D \cos(\omega_D t + \delta_D)$  applied to the flat endcaps of our model of a linear ion trap is [20]

$$\begin{aligned} \phi_{ends}(x, y, z, t) &= \kappa [U_D + V_D \cos(\omega_D t + \delta_D)] \left[ \frac{z^2}{z_0^2} - \frac{x^2 + y^2}{2z_0^2} \right], \end{aligned} \quad (17)$$

where the parameter  $\kappa$  depends on the trap geometry and must be determined experimentally or by solution of the Laplace equation for a particular trap. Differentiating equations (16) and (17) with respect to  $x$  gives the electric field in the  $x$  direction and similarly for  $y$  and  $z$ . After some algebraic manipulation, the results can be put in a form like equation (13), with the values of the tilde quantities given in Table 2 in terms of the quantities without tildes defined above.

Table 1: Dimensionless quantities characterizing the moment equations for stretched or non-ideal quadrupole ion traps.

Quantity	Value for stretched or non-ideal quadrupole ion trap
$\tilde{a}_x$	$a_x \left( -\frac{r_0^2+2z_0^2}{2r_0^2} \right) \left[ A_2 + A_4 \frac{12z^2-3(x^2+y^2)}{2r_0^2} + A_6 \frac{120z^4-1880z^2(x^2+y^2)+15(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{a}_y$	$a_y \left( -\frac{r_0^2+2z_0^2}{2r_0^2} \right) \left[ A_2 + A_4 \frac{12z^2-3(x^2+y^2)}{2r_0^2} + A_6 \frac{120z^4-1880z^2(x^2+y^2)+15(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{a}_z$	$a_z \left( -\frac{r_0^2+2z_0^2}{2r_0^2} \right) \left[ A_2 + A_4 \frac{2z^2-3(x^2+y^2)}{r_0^2} + A_6 \frac{24z^4-120z^2(x^2+y^2)+45(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{q}_x$	$q_x \left( -\frac{r_0^2+2z_0^2}{2r_0^2} \right) \left[ A_2 + A_4 \frac{12z^2-3(x^2+y^2)}{2r_0^2} + A_6 \frac{120z^4-1880z^2(x^2+y^2)+15(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{q}_y$	$q_y \left( -\frac{r_0^2+2z_0^2}{2r_0^2} \right) \left[ A_2 + A_4 \frac{12z^2-3(x^2+y^2)}{2r_0^2} + A_6 \frac{120z^4-1880z^2(x^2+y^2)+15(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{q}_z$	$q_z \left( -\frac{r_0^2+2z_0^2}{2r_0^2} \right) \left[ A_2 + A_4 \frac{2z^2-3(x^2+y^2)}{r_0^2} + A_6 \frac{24z^4-120z^2(x^2+y^2)+45(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{b}_x$	$b_x \left( -\frac{r_0^2+2z_0^2}{4r_0^2} \right) \left[ 6A_3 + A_5 \frac{20z^2-15(x^2+y^2)}{r_0^2} + \dots \right]$
$\tilde{b}_y$	$b_y \left( -\frac{r_0^2+2z_0^2}{4r_0^2} \right) \left[ 6A_3 + A_5 \frac{20z^2-15(x^2+y^2)}{r_0^2} + \dots \right]$
$\tilde{b}_z$	$b_z \left( -\frac{r_0^2+2z_0^2}{4r_0^2} \right) \left[ A_1 + A_3 \frac{6z^2-3(x^2+y^2)}{r_0^2} + A_5 \frac{40z^4-120z^2(x^2+y^2)+15(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{d}_x$	$d_x \left( -\frac{r_0^2+2z_0^2}{4r_0^2} \right) \left[ 6A_3 + A_5 \frac{20z^2-15(x^2+y^2)}{r_0^2} + \dots \right]$
$\tilde{d}_y$	$d_y \left( -\frac{r_0^2+2z_0^2}{4r_0^2} \right) \left[ 6A_3 + A_5 \frac{20z^2-15(x^2+y^2)}{r_0^2} + \dots \right]$
$\tilde{d}_z$	$d_z \left( -\frac{r_0^2+2z_0^2}{4r_0^2} \right) \left[ A_1 + A_3 \frac{6z^2-3(x^2+y^2)}{r_0^2} + A_5 \frac{40z^4-120z^2(x^2+y^2)+15(x^2+y^2)^2}{8r_0^4} + \dots \right]$
$\tilde{f}_x$	$\frac{xz}{r_0}$
$\tilde{f}_y$	$\frac{yz}{r_0}$
$\tilde{f}_z$	$r_0$

### 4. Moment Equations for Traps

When equation (13) is inserted into equation (1), the moment equation for  $\bar{v}_u$  in stretched or nonideal quadrupole traps and in linear traps can be written in the same form:

$$\frac{\partial}{\partial t} \bar{v}_u + \frac{\Omega_{RF}^2}{4} [\tilde{a}_u - 2\tilde{q}_u \cos(\Omega_{RF}t)] u + \frac{\Omega_{RF}^2}{4} [\tilde{b}_u - 2\tilde{d}_u \cos(\omega_D t + \delta_D)] \tilde{f}_u + \xi_u \bar{v}_u = 0. \tag{18}$$

The important new thing about this result is that it applies both to linear traps and (when we set  $\tilde{a}_u = a_u$ ,  $\tilde{q}_u = q_u$ , and  $\tilde{b}_u = \tilde{d}_u = 0$ ) to ideal quadrupole ion traps, and in all four of the moment theories discussed above.

For the 2T and SB theories, equation (2) is simplified by introducing the dimensionless temperature:

$$\varepsilon = \frac{T_{\text{eff}}}{T}. \tag{19}$$

This quantity is also equal to the ratio of the average energy of the collision between an ion and a buffer gas molecule to the thermal energy of the gas. It is always greater than 1 because the electric fields always act to increase the collision energy.

When equations (2) and (19) are used with equation (13), we get

$$\begin{aligned} \frac{\partial}{\partial t} \varepsilon + \frac{\mu \Omega_{rf}^2}{6k_B T} & \times \sum_{u=x,y,z} [\tilde{a}_u - 2\tilde{q}_u \cos(\Omega_{RF}t)] u \bar{v}_u \\ & + \frac{\mu \Omega_{rf}^2}{6k_B T} \sum_{u=x,y,z} [\tilde{b}_u - 2\tilde{d}_u \cos(\omega_D t + \delta_D)] \tilde{f}_u \bar{v}_u \\ & + \frac{2\mu \xi}{M} \left[ \varepsilon - 1 + \frac{M\Phi}{m} \varepsilon \right] = 0. \end{aligned} \tag{20}$$

The important thing is that equations (18) and (20) constitute a set of four coupled, ordinary differential equations describing the ion motion in ideal and nonideal quadrupole ion traps, or in linear traps, according to the first approximation of the 2T and SB theories. To study ion-neutral reactions in the 2T theory, one must also solve equation (4), use the ion motion results in equation (5), and then perform the integral in equation (7).

For the MT and CB theories, we introduce a dimensionless effective temperature along each direction. Thus

$$\varepsilon_u = \frac{T_{u,\text{eff}}}{3T}, \tag{21}$$

Table 2: Dimensionless quantities characterizing the moment equations for linear ion traps.

Quantity	Value for Linear Ion Trap
$\tilde{a}_x$	$a_x \left( \frac{r_0^2 + 2z_0^2}{r_0^2} \right) \left[ A_2 + A_6 \frac{3x^4 - 30x^2y^2 + 15y^4}{r_0^4} + \dots \right]$
$\tilde{a}_y$	$a_y \left( -\frac{r_0^2 + 2z_0^2}{r_0^2} \right) \left[ A_2 + A_6 \frac{3y^4 - 30y^2x^2 + 15x^4}{r_0^4} + \dots \right]$
$\tilde{a}_z$	0
$\tilde{q}_x$	$q_x \left( \frac{r_0^2 + 2z_0^2}{r_0^2} \right) \left[ A_2 + A_6 \frac{3x^4 - 30x^2y^2 + 15y^4}{r_0^4} + \dots \right]$
$\tilde{q}_y$	$q_y \left( -\frac{r_0^2 + 2z_0^2}{r_0^2} \right) \left[ A_2 + A_6 \frac{3y^4 - 30y^2x^2 + 15x^4}{r_0^4} + \dots \right]$
$\tilde{q}_z$	0
$\tilde{b}_x$	$b_x \left( -\frac{r_0^2 + 2z_0^2}{2z_0^2} \right) \kappa$
$\tilde{b}_y$	$b_y \left( -\frac{r_0^2 + 2z_0^2}{2z_0^2} \right) \kappa$
$\tilde{b}_z$	$b_z \left( -\frac{r_0^2 + 2z_0^2}{2z_0^2} \right) \kappa$
$\tilde{d}_x$	$d_x \left( -\frac{r_0^2 + 2z_0^2}{2z_0^2} \right) \kappa$
$\tilde{d}_y$	$d_y \left( -\frac{r_0^2 + 2z_0^2}{2z_0^2} \right) \kappa$
$\tilde{d}_z$	$d_z \left( -\frac{r_0^2 + 2z_0^2}{2z_0^2} \right) \kappa$
$\tilde{f}_x$	$x$
$\tilde{f}_y$	$y$
$\tilde{f}_z$	$z$

where the factor of 3 is introduced so that  $\varepsilon_x + \varepsilon_y + \varepsilon_z$  becomes equal to  $\varepsilon$  when the three ion temperatures are identical, and the MT and CB theories reduce to the 2T and SB theories, respectively. Then equations (3), (13), and (21) give

$$\begin{aligned} \frac{\partial}{\partial t} \varepsilon_u + \frac{\mu \Omega_{rf}^2}{6k_B T} [\tilde{a}_u - 2\tilde{q}_u \cos(\Omega_{RF}t)] u \bar{v}_u \\ + \frac{\mu \Omega_{rf}^2}{6k_B T} [\tilde{b}_u - 2\tilde{d}_u \cos(\omega_D t + \delta_D)] \tilde{f}_u \bar{v}_u \quad (22) \\ + \frac{2\mu \xi_u}{M} \left[ \varepsilon_u - \frac{1}{3} + \frac{M \Phi_u}{m} \varepsilon_u \right] = 0. \end{aligned}$$

The important thing is that equations (18) and (22) represent six coupled, ordinary differential equations completely describing the ion motion in ideal and nonideal quadrupole ion traps, or in linear traps, according to the first approximation of the MT and CB theories. To study ion-neutral reactions in the MT theory, one must also solve equation (4), use the ion motion results in equation (8), and then perform the integral in equation (7).

We have written computer programs in Mathematica and in Fortran to solve the first-order moment equations, using the SB and MT theories. The advantage of the Mathematica program is that the numerical details of how the coupled differential equations are solved are left to the software. In contrast, the advantage of the Fortran program is that

the method of solution is completely specified (fourth-order Runge-Kutta) and the programmer has more control over the level of numerical accuracy. The Fortran program generally runs in less time on a Sun workstation than the Mathematica program requires on a Dell computer, but each program takes only on the order to 15–60 minutes, depending upon the choices made for the parameters of the ion trap, the initial conditions, and so forth. A copy of either program can be obtained from the authors.

## 5. Tests

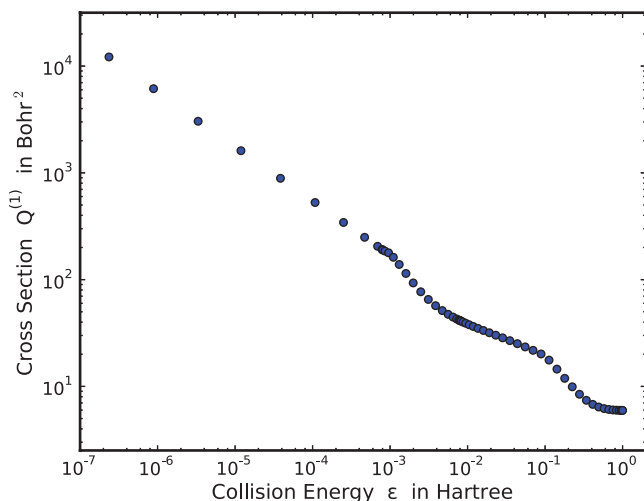
Before using our new programs for linear traps, however, it is important that we verify that they reproduce the previous results for ideal and stretched quadrupole traps. The Maxwell model of constant collision frequency corresponds to an ion-neutral interaction potential that varies inversely with the fourth power of the separation between the colliding particles. Since this describes the attractive interaction potential at very large separations between any atomic ion and an atom in an  $s$  state, the Maxwell model is generally regarded as a good one to use for atomic systems when both the gas temperature and electric field strength are small. In addition,  $\xi_u$  is the same constant for all directions  $u$ , regardless of whether the 2T or MT theory is used, while  $\Phi = 0$  for the SB theory and

$$\Phi_u = \frac{1}{2} \left[ 1 - \frac{\varepsilon_x + \varepsilon_y + \varepsilon_z}{3\varepsilon_u} \right] \quad (23)$$

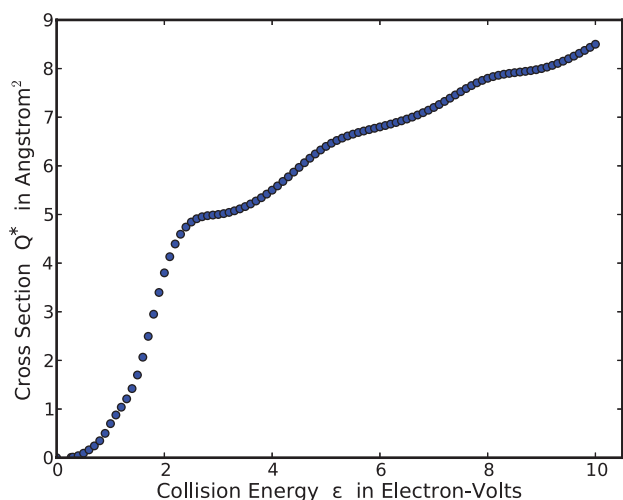
for the MT theory. The results obtained from the new computer programs have been checked for Maxwell molecules against those given in Figures 1 and 2 of [3] for the ideal quadrupole trap; they agree to three significant figures or more.

We also considered a stretched quadrupole ion trap using the Maxwell model for collisions between singly charged ions with  $m = 100$  Da and neutral atoms with  $M = 4$  Da,  $T = 300$  K, and  $\xi_u = 740.9 \text{ s}^{-1}$ . We focused on the steady-state velocities by assuming that the average initial velocities are zero in all three directions and that the initial value of  $T_{u,\text{eff}}$  is  $T$  in all directions. We also assumed that the ion trap operates with no dc field on the rods ( $\tilde{a}_u = 0$ ), no ac or dc field on the endcaps ( $\tilde{b}_u = \tilde{d}_u = 0$ ), and with an ac field on the ring such that  $\tilde{q}_x = \tilde{q}_y = -0.10$ ,  $\tilde{q}_z = 0.20$ , and  $\Omega_{RF}/2\pi = 1.0$  MHz. These choices are exactly those used previously [6] for an ideal quadrupole trap, and our results from both programs agree to 3 significant figures with those in Figures 1–2 of [6].

A rigid-sphere interaction is often used to model collisions at very high energy. To test our programs in this case we used  $m = 100$  Da,  $M = 4$  Da,  $T = 300$  K,  $P = 0.001$  torr, a constant cross section of  $50 \text{ \AA}^2$ ,  $\Omega_{RF}/2\pi = 1.00$  MHz,  $a_z = 0.0010$ ,  $a_x = a_y = -0.0005$ ,  $q_z = 0.2500$ , and  $q_x = q_y = -0.1250$ . The initial velocities were chosen as in [3], and we obtained the same values for ideal quadrupole traps shown in Figures ??–?? of that paper.



**Figure 1:** Momentum-transfer cross section,  $Q^{(1)}(\epsilon)$ , in square bohr (1 bohr =  $0.52917721092 \times 10^{-10}$  m) as a function of the collision energy,  $\epsilon$ , in hartree (1 hartree =  $4.35974434 \times 10^{-18}$  J) for  $^{16}\text{O}^+(^4\text{S}^0)$  ions interacting with Ar atoms.



**Figure 2:** Total reaction cross section,  $Q^*(\epsilon)$ , in square Angstrom (1 Angstrom =  $1.0 \times 10^{-10}$  m) as a function of the collision energy,  $\epsilon$ , in eV (1 eV =  $1.602176565 \times 10^{-19}$  J) for  $^{16}\text{O}^+(^4\text{S}^0)$  ions reacting with  $\text{N}_2$  molecules.

We also considered a stretched quadrupole ion trap using the rigid sphere model for the ion-neutral collisions. Using the same parameters as in [6], we obtained MT results that matched those given previously [6]. Specifically, both of our new computer programs gave values of the ion velocity along  $z$  as 3.14 km/s and the effective temperature along  $z$  as 4.86 kK (4860 K, to three significant figures) at the first peak of the ac field,  $0.250 \mu\text{s}$ , after the start of the simulation.

Finally, we considered the reaction rate coefficient between  $^{107}\text{Ag}^+$  and  $\text{D}_2$  in an ideal quadrupole trap containing He in a much larger amount than  $\text{D}_2$ . The conditions were the same as in [8], which reported the first *ab initio*

calculation of the reaction rate coefficient in a trap; that is, it was based on an *ab initio* potential energy curve for the interaction of the ions and rare gas atoms. The present values for the rate coefficient averaged over one period of the ac field and over all positions in the trap were within 4% of each other and of the previous value [9],  $4.78 \times 10^{-15} \text{ cm}^3/\text{s}$ . The differences are due to the numerical techniques used to evaluate equation (5); although they can be eliminated by letting the programs run longer with more elaborate quadrature techniques, they are smaller already than errors ordinarily expected for ion-neutral reaction rate coefficients in drift tubes, ion traps, and so forth. Unfortunately, this predicted value is smaller than the lower limit for determining reaction rate coefficient in ion traps, so no experimental values are available to compare with. The reason for this small value is that the reaction cross section has a threshold at energies substantially above thermal values.

## 6. New Applications

As a new application of our computer programs, we consider  $^{16}\text{O}^+(^4\text{S}^0)$  moving in a linear ion trap through Ar at 300.0 K and 0.01000 torr; four significant figures were used here and in all of the other parameters cited below, in order to be consistent. It has been shown previously [21] that the appropriate potential for the description of the motion of this ion through Ar at the energies of interest in experiments conducted in drift-tube mass spectrometers and ion traps is the diabatic potential, neglecting fine structure. By using an accurate  $^4\Sigma^-$  potential between 2.08 and 30.24 bohr for the  $\text{O}^+$ -Ar system, agreement with the mobility measurements [21] was obtained for low and intermediate values of  $E/N$ , although small discrepancies remained for high values. Since no potential energy curves of higher accuracy appear to have been calculated since 2008, we have used this potential to determine the momentum-transfer cross section with an accuracy of 0.1% over energies from  $10^{-9}$  to 10 hartree, using program PC [22]. The results are shown in Figure 1. Note that  $Q^{(1)}$  is not constant, like it would be for a rigid-sphere action, nor does it decrease linearly (with a slope of  $-1/2$ ) on this log-log plot, like it would for the Maxwell model.

For the total reaction cross section between  $^{16}\text{O}^+(^4\text{S}^0)$  ions and  $\text{N}_2$  molecules (in equilibrium with the Ar atoms in which they compose only 0.1000% of the total particles), we use the values between 0.3 and 10 eV of Albritton et al. [23]. The reaction products are  $\text{NO}^+$  and N. The cross section values are shown in Figure 2.

For the MT applications described here, we used  $r_0 = 1.000$  cm, which means that the  $r = 1.126$  cm. We assumed that  $z_0 = 5.000$  cm, which means that the total length of the trap was 10.000 cm. The trap was assumed to have  $\kappa = 1.000$ ,  $A_2 = 1.001462$ ,  $A_6 = 0.001292$ , and  $A_{10} = -0.002431$ . There was assumed to be an ac field of frequency  $\Omega_{RF}/2\pi = 1.000$  MHz on the rods, but no dc field on the rods and no electrical field of either type on the endcaps. We used  $q_x =$

–0.1000 and studied 4 positions between 0 and 1.420 mm along both  $x$  and  $y$ , but 4 positions between 0 and 0.7100 mm along  $z$ . We assumed that the initial ion distributions had a normal distribution in space with  $\sigma_x = \sigma_y = 0.7100$  mm and  $\sigma_z = 0.3550$  mm. The simulations generally involved 50 time steps for each 1.000  $\mu$ s, although we did make a limited number of calculations using 100 time steps that did not produce significant differences. Steady-state behavior was established by comparing the set of ion velocities and temperatures at the end of a cycle of the  $rf$  field with those used at the start of the calculations.

We made calculations with two sets of initial conditions. The first had initial velocities of 395.3 m/s along  $x$ , –395.3 m/s along  $y$ , and 350.0 m/s along  $z$ . It had initial temperature (energy) ratios of 1.000 along each axis, so each  $\epsilon_u$  was set equal to 1/3 initially. Averaging the results over 2.5 cycles of the field (2.5  $\mu$ s) and all positions in space gave a reaction rate coefficient of  $6.12 \times 10^{-13}$  cm<sup>3</sup>/s with the Fortran code and  $6.52 \times 10^{-13}$  cm<sup>3</sup>/s with the Mathematica code. The second simulation used initial velocities of 0 but temperature ratios of 1.4527 along  $x$  and  $y$  and 0.99230 along  $z$ ; the average reaction rate coefficients were  $6.61 \times 10^{-13}$  cm<sup>3</sup>/s and  $6.40 \times 10^{-13}$  cm<sup>3</sup>/s. These values could be improved by using more values for the positions, putting more time steps per cycle, and using simulation times long enough so that the choice of initial conditions becomes unimportant. Nevertheless, the values are sufficiently close to conclude that the average reaction rate coefficient could be measured in linear traps that currently exist.

Because  $q_x$  is inversely proportional to the ion mass, the value of –0.1 used in the preceding calculations is not as small as what might be assumed by researchers more accustomed to studying large ions in traps. At  $x = y = z = 1.0$  mm, the collision energies in these calculations reached values as large as  $\epsilon_x = \epsilon_y = 4.9$  and  $\epsilon_z = 2.0$ , equivalent to 0.38 and 0.16 eV, respectively. At  $x = y = z = 2.00$  mm, the values were as large as  $\epsilon_x = \epsilon_y = 9.8$  and  $\epsilon_z = 3.8$ , or 0.76 and 0.29 eV. We performed an additional set of calculations with  $q_x = -0.2000$  and found that the collision energies at  $x = y = z = 1.0$  mm reached values as large as  $\epsilon_x = \epsilon_y = 9.7$  and  $\epsilon_z = 3.8$ , equivalent to 0.75 and 0.29 eV, respectively; at  $x = y = z = 2.00$  mm, they were as large as  $\epsilon_x = \epsilon_y = 19.3$  and  $\epsilon_z = 7.3$ , or 1.50 and 0.57 eV. Larger values of the dimensionless field parameters would reach collision energies above those for which the cross section for  $^{16}\text{O}^+$  reactions with  $\text{N}_2$  is known.

## 7. Conclusions

We have extended the previous moment theories for ion motion and reaction so that they apply to linear traps as well as ideal and stretched quadrupole traps. Fortran and Mathematica computer programs have been written to implement the first approximation moment equations. These programs have been checked against one another and against

previous results obtained for quadrupole traps. They were then used to predict the reaction rate coefficients that would be measured when  $^{16}\text{O}^+(^4\text{S}^0)$  ions move through Ar gas in which there is 0.1% of  $\text{N}_2$ . Taking into account possible errors due to using only the first approximation moment equations and the differences observed with the different computer programs, the predicted values are  $6.4 \pm 0.9 \times 10^{-13}$  cm<sup>3</sup>/s when the trap parameters are as given above. The error estimate would have to be increased if the reactive cross sections used here were found to be inaccurate. The important point, however, is that this value is sufficiently large that the average rate coefficient should be measurable in a linear ion trap.

The computer programs described here can be used for many ion-neutral systems. The first requirement is that information should be available about the energy dependence of the momentum-transfer cross section between the ion of interest and some inert, buffer gas (typically He or Ar). *Ab initio* results are available from the authors for just over 50 atomic ions and a few molecular ions; eventually we hope to add these values to the on-line database [24] that already contains the potentials from which they can be determined and the transport coefficients that depend upon them (and other transport cross sections). The second requirement is information about the dependence of the total reaction cross section as a function of the energy of collision between the ion and some reactive molecule. *Ab initio* calculations of these cross sections are becoming feasible, although it may be necessary to work with model cross sections, particularly if one is interested in large molecules. The third requirement is precise information about the values of the many quantities (e.g., ac frequencies, electric field strengths, and trap parameters) that are used in the experiments.

In most cases, the least well known of the three things listed above are the reaction cross sections. These are the fundamental quantities, as opposed to the reaction rate coefficients that can change considerably with even slight changes in experimental conditions. We look forward to working with an experimental group to combine theoretical information about the momentum-transfer cross section with experimental information about ion traps in order to infer total reaction cross sections.

## Acknowledgments

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## Appendix A: Collision Frequencies

In the MT theory, the collision frequencies,  $\xi_u$ , depend upon three effective temperatures, one along each Cartesian axis  $u$ . They are given by equations (74)–(76) of [1] as



$$\xi_u(T_{x,\text{eff}}, T_{y,\text{eff}}, T_{z,\text{eff}}) = \frac{8N\mu}{3m} \left( \frac{2k_B T}{\pi\mu} \right)^{1/2} \langle \gamma_u^2 \rangle^{(1)}, \tag{A1}$$

where

$$\langle A \rangle^{(l)} = \frac{3}{4\pi} \iiint_{-\infty}^{\infty} \exp(-\gamma_x^2 - \gamma_y^2 - \gamma_z^2) g Q^{(l)}(g^2 k_B T) A d\gamma_x d\gamma_y d\gamma_z \tag{A2}$$

and

$$g^2 = \gamma_x^2 \frac{T_{x,\text{eff}}}{T} + \gamma_y^2 \frac{T_{y,\text{eff}}}{T} + \gamma_z^2 \frac{T_{z,\text{eff}}}{T}. \tag{A3}$$

(It should be noted that there are two factors of 3 missing in the form of these equations given by equation (A.4) of [6], which arose from oversight of the factor of 3 in equation (13) of that paper.) The momentum-transfer cross section,  $Q^{(1)}$ , is one of a family of transport cross sections that can be accurately calculated [22] from knowledge of the interaction potential energy curve for the atomic ion-atom pair.

For quadrupole ion traps, the strict cylindrical symmetry of the apparatus guarantees that the  $x$  and  $y$  effective temperatures are the same. This means that (A2) may be expressed in cylindrical polar coordinates and then simplified to a two-dimensional integral. This simplified form was implemented in the computer program used in previous calculations [7, 8]. It is important to note that this simplification guarantees that the computer programs will run much faster for quadrupole traps than for linear traps.

The essence of the 2T theory is to assume that all three effective temperatures are the same. In this case, equation (A1) simplifies to

$$\xi(T_{\text{eff}}) = \frac{8N\mu}{3m} \left( \frac{2k_B T_{\text{eff}}}{\pi\mu} \right)^{1/2} \times \int_0^\infty \exp(-\gamma^2) Q^{(1)}(\gamma^2 k_B T_{\text{eff}}) \gamma^5 d\gamma. \tag{A4}$$

Extensions of equations (A1) and (A3) that apply to the SB and CB theories of molecular ion-neutral systems are given in the appendix of [6] and so need not be repeated here.

For classical-mechanical collisions between rigid spheres of diameter  $d$ , the momentum-transfer cross section is independent of energy. Thus

$$Q^{(1)} = \pi d^2. \tag{A5}$$

Although the collision frequencies still depend upon the effective temperature(s), the constant cross section simplifies equations (A1) and (A4) and greatly increases the speed of both MT and 2T computer programs—at the cost of a poorer description of the physics of the collisions.

A different simplification arises for the Maxwell model, where  $gQ^{(1)}(g^2 k_B T)$  is constant. In this case, the collision frequencies are constant, as assumed in the Mathieu equation for ion traps. This model is perfect for ion-neutral interaction potentials that vary as the inverse-fourth power of the separation, which correctly describes most ion-neutral interactions at very large separation. This in turn makes it a valid model at low temperature, where most collisions occur at large separations. Unfortunately, we now know that such temperatures must be below (and sometimes far below) 1 K. In short, the Maxwell model can also greatly increase the speed of MT and 2T computer programs, but again at the cost of a poorer description of the physics of the collisions at the usual temperatures employed with ion traps.

## Appendix B: The $\Phi$ The Quantities

The  $\Phi$  quantities that arise in the various moment theories of ion traps are dimensionless ratios of collision integrals. They account for energy partitioning among the three Cartesian directions and, in the case of molecular ions and neutrals, between translational and internal degrees of freedom. For the 2T theory,  $\Phi = 0$ . For the MT theory, it has been shown [6] that

$$\Phi_u = \frac{\langle 3T_{u,\text{eff}}\gamma_u^2 - T_{x,\text{eff}}\gamma_x^2 - T_{y,\text{eff}}\gamma_y^2 - T_{z,\text{eff}}\gamma_z^2 \rangle^{(2)}}{6 \langle T_{u,\text{eff}}\gamma_u^2 \rangle^{(1)}}. \tag{B1}$$

For the other theories, the expressions are given in the Appendix of [6].

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Although publications covering various aspects of nuclear receptors (NRs) appear every year in high impact journals, these publications are virtually buried among an overwhelming volume of articles that are only peripherally related to NRs. The latter fact prompted a group of prominent scientists active in the field of nuclear receptor research to conclude that gathering publications on this superfamily of receptors under one umbrella would provide an invaluable resource for a broad assemblage of scientists in the field; thus the idea for a new journal, **Nuclear Receptor Research**, was born.

I am pleased to share with you that **Nuclear Receptor Research** is now a reality as an open access peer-reviewed journal devoted to publishing high-quality, original research and review articles covering all aspects of basic and clinical investigations involving members of the nuclear receptor superfamily. **Nuclear Receptor Research** has an editorial board comprised of a group of renowned scientists from around the world. Board members are committed to make **Nuclear Receptor Research** a vibrant forum showcasing global efforts in this ever-expanding area of research.

We believe that the impact and visibility of papers related to nuclear receptors will be significantly enhanced by appearing in a journal devoted exclusively to nuclear receptors. In addition, it is hoped that **Nuclear Receptor Research** will serve as a catalyst to encourage collaborative studies as well as to foster interdisciplinary initiatives within this expansive and dynamic field. For these reasons, I invite you to consider **Nuclear Receptor Research** (<http://www.agialpress.com/journals/nrr/>) as a vehicle to share your novel research findings as well as your vision for the future of nuclear receptor research with your colleagues around the world.

Mostafa Badr  
Editor-in-Chief  
**Nuclear Receptor Research**