1)01'1'1 ER SIDEBAND SPECTRA FOR 10NS IN A LINEAR TRAP[1]

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Abstract

We describe a spectroscopic measurement of the temperatu re and linear density of Hg^+ ions held in a linear ion trap (LIT). The infer ed temperature and number result from analysis of sidebands on the 40.5 GHz resonance line. The temperature of the ion cloud is determined by 'the Doppler broadened line when microwave radiation is propagated along the axis of the 1,1'1". When propagation is perpendicular 10 the trap axis the microwave sidebands arc displaced from the trap secular frequency by an amount dependent upon the ion cloud size and tem perature. A Monte-Carlo simulation of the ion trajectories inside the cloud is used to mode] the.position of these sidebands for a given cloud temperature and a comparison with measured sideband position is used to determine ion number.

Introduction

One of the largest frequency offsets in lamp based buffer gas cooled Mercury ion frequency standards is the second order Doppler shift from the. thermal and micro-motion of the. ions within the trap[1,2]. At room temperature with Hg^+ ions in a 1 .] 'J' this shift is $(1+2/3)3k_BT/(2mc^2) = 3.5\times10^{-13}$ for a small cloud where space charge screening of the time averaged trapping field is negligible. In Ibis case a measurement of ion cloud temperature accurate to 10% would yield a room temperature I Ig clock with accuracy at few parts in 10^{14}, approaching that of the best primary Cesium standards currently in operation. 'l-his paper describes temperature measurements and ion number determination for ion clouds held in a linear ion trap. Such measurements are necessary to assess clock frequency offset from the 2nd order 1 Doppler shift and to determine clock accuracy[3]. Kllcm'ledge of cloud size and temperature also se rves as a useful diagnostic of ion trap operation.

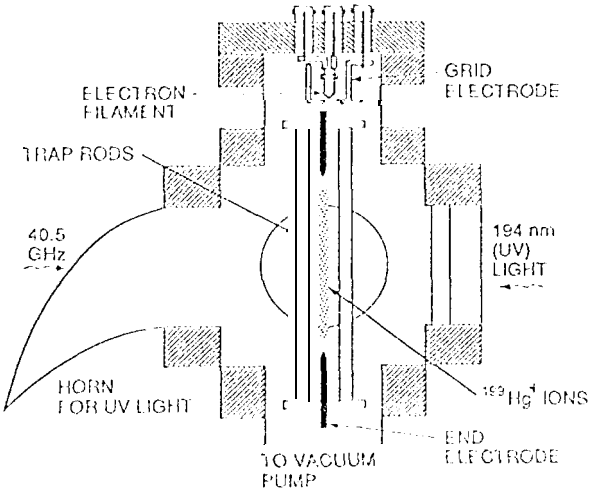

Figure 1: Linear ion trap residing in its high vacuum enclosur c. Stale selection light from the ^{202}Hg discharge lamp is focused onto the central 1/3 of the of the ion cloud. Atomic fluorescence is collected normal to the page.

[1] This work represents one phase of research carried out at the Jet Propulsion Laboratory, California Institute of Technology, under contract to the National Aeronautics and Space Administration.

Figure 1 shows the present I .1'1' configuration as used in clock operation[4]. Ions arc confined in the cylindrical cloud up 10 75 mm in length by a few mm in diameter. An ion's thermal motion inside the cloud will lead to a high frequency secular motion corresponding to transit across the fcw mm cloud diameter and a much lower frequency Corresponding to axial motion along the approximately 7S mm long cloud, When there arc only a few ions in the trap the resultant forces on the ions arc predominately from the trapping fields. The transverse motion is then harmonic and all ions undergo motion at the secular frequency of the trap. As the 40. S GIIz radiation propagates radially through the cloud an ion's motion in the trap will modulate the phase of the microwaves. This results in sidebands on the atomic absolution spectrum of fset from the 40. S GIIz carrier by the trap secular frequency and its harmonics. As more ions are added 10 the trap the cumulative effect of the trapped charges begins 10 shield the lime averaged trapping fields from the interior of the ion cloud. Ions moving inside the cloud will no longer fee] the harmonic trapping well and the result is a broadened and downshifted Doppler sideband spectrum. We have computed the spectrum of microwave power seen by an ion moving through the cloud by a Monte-Carlo sampling of ion trajectories and the resulting phase variation. For a fixed cloud temperature the Doppler sideband shifts downward monotonically with increasing number of trapped ions. Once the ion temperature has been measured the cloud size. is determined by adjusting ion number until the simulated and measured sideband frequencies match.

Ion Temperature Measurement

We measure. ion temperature spectroscopically by propagating the 40.5 GIIz resonance radiation along the 75mm long axis of the ion cloud, In this configuration ion confinement is 10 times the wavelength of the 7,5 mm resonance radiation and the Doppler width of the 40.5 Ghz absorption line is used to determine the cloud temperature[5]. Because the 50 mini-gauss bias field is parallel to this axis of the trap and hence perpendicular to the oscillating magnetic field of the microwave radiation, the allowed transitions obey $\Delta m_F = \pm 1$. These transitions arc from the $F=0, m_F=0$ state. to the $F=1, m_F=+1$ Zeeman slates. Figure 2 shows the Doppler broadened microwave lines obtained by propagating microwaves along this direction. 'J he width of the microwave transition is $\delta\nu = 2(v_0/c)(2k_B T \cdot \ln 2/m)^{1/2} = 2.056 T^{1/2}$ kIIz [6], where 'r is temperature in Kelvin. The 46 kHz wide spectral lines in Fig. 2 indicate an ion cloud temperature of S00 K. By use of this technique we have measured ion cloud temperature variations with helium buffer gas pressure. As shown in Figure 3 the ion temperature varies from 2610 K at 2×10^{-8} Torr (uncorrected) to 480 K at 7×10^{-6} Torr (uncorrected). For the clouds used in our clock measurements Helium pressures above 2×10^{-6} Torr (uncorrected) are necessary for minimum temperatures.

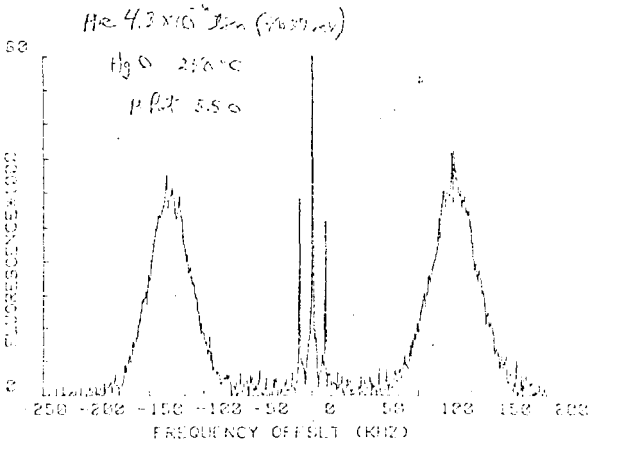

Figure 2: The Doppler broadened Zeeman hyperfine transitions $F=0, m_F=0$ to $F=1, m_F=\pm 1$ which are Used to determine the Hg^+ temperature. For Ibis measurement the 40.5 GIIz radiation passed axially through the 75 mm long cloud.

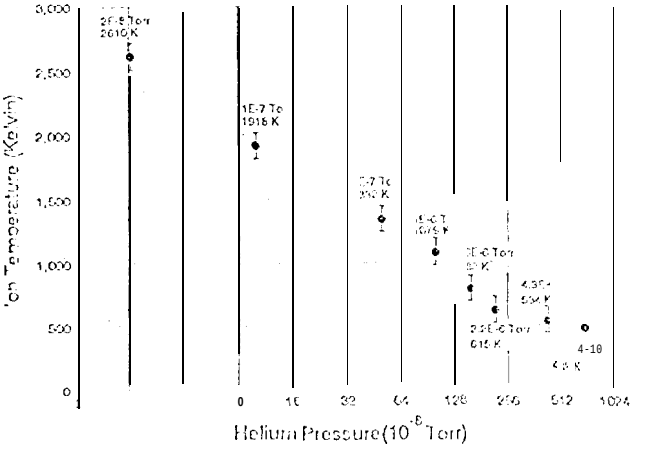

Figure 3: Hg^+ cloud temperature vs helium buffer gas pressure as determined from the doppler width of the 40.5 GIIz transition.

Transverse Microwave Excitation of Ion Cloud

By propagating the 40.5 GHz resonance radiation perpendicular to thelong axis of the ion cloud we can investigate the absorption sidebands which stem from the high frequency secular ion motion across the. cloud diameter. The measured resonance structure is shown in Figure 4 (a) and (b). In Fig. 4(a) the helium pressure is $5x10^{-8}$ Torr (uncorrected) so ion temperature is over 2000 K. The calculated secular frequency at the

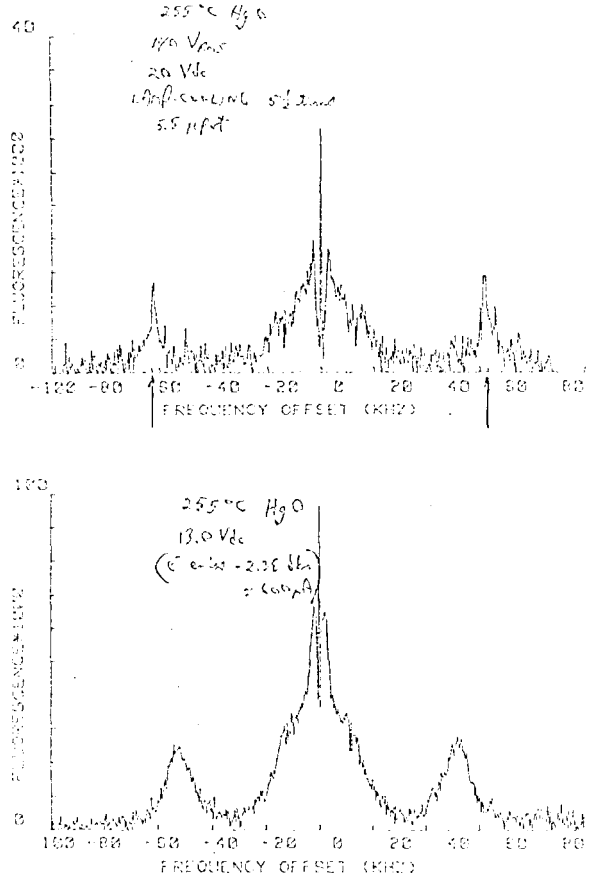

Figure 4: Sideband spectra obtained by transverse microwave illumination of the ion cloud as shown in Fig. 1. (a) Low helium buffer pressure and resulting ion temperature over 2000 K. Sidebands Snow' very little shift from the. 62 kHz trap secular frequency. (b) Sidebands shift by 10 kHz as the helium pressure is increased and ion temperature falls to 650 K.

operating rf voltage level (140 Volts rms @ 853 k] Iz) is 62 kHz and is in good agreement with the frequency of the transverse sidebands. This indicates low ion density since there is no significant screening of the trapping fields by the ion space charge. By contrast Fig. 4(b) shows that the sidebandshave shifted closer to the 40.5 GHz carrier by about 10 kHz as the helium pressure was il~cl-cased to 2x10"6 Torr (uncorrected). The signal size has also quadrupled since many more ions are trapped under these conditions.

Monte-Carlo calculation of Sideband Frequencies

The approach used in predicting the. frequency of the secular sidebands as described above is to determine the microwave frequency spectrum seen by an ion inside the cloud[7]. A spherical wavefront is incident on the ion cloud from a distance R_0. The magnetic field seen by an ion at position r at time t is

$$B(r,t) = B_0 \exp[i(k_{\mu w} r - \omega t)]/(k_{\mu w} r)$$

where $k_{\mu w} = 2\pi/\lambda_{\mu w}$ and $\lambda_{\mu w}$ is the wavelength of the microwave radiation, ≈7.5 mm. The ions are in thermal motion inside the cloud so that r = r(t) and the. spherical wave is modulated by the individual ion motions. This motion is determined by the velocity distribution and the shape of the ioncloud. The long thin cloud leads to microwave modulation frequencies of order v_{mp}/D and v_{mp}/l, u'here v_{mp} is the most probable velocity for the ions at temperature 'T', D is the cloud diameter and 1, is the cloud length. The power spectral density of (he. 40. S GHz radiation as seen by the ensemble of confined moving ions is related to the autoco I relation function of the. microwave magnetic field through the cosine transform (Wiener-Khintchine Theorem)

$$P(\omega) = \int d\tau \psi(\tau) \cos\omega\tau$$

where $\psi(\tau)$ is the autocorrelation function

$$\psi(\tau) = B_0^2 Re[\exp(-ik_{\mu w}(r(\tau)-r(0))/(k_{\mu w}^2 r(0) r(\tau))]$$

The averaging is to be carried out over the ionic trajectories through the cloud. To generate this average a set of initial conditions consistent with the velocity and position distribution functions is chose II with a trajectory being generated through the potentials seen inside the cloud. Ignoring collisions, an ion moves in response to the space charge potential of the other ions and the harmonic trap potential. The

starting point is calculation of the density profile for a given number of ions at temperature T in a cylindrically symmetric harmonic trapping well of secular frequency ω [8]. The ion cloud is assumed to be of uniform linear density Up to the ends of the trap.

Boltzmann Density Profile

We assume that the. ion cloud is in thermal equilibrium at temperature '1' so that the ion number density n(ρ) satisfies a Boltzmann distribution [7]

$$n(\rho) = n(0)\exp[-\Phi_{total}(0)/kT]$$

where $\Phi_{total}(\rho) = m\omega^2\rho^2/2 + q\varphi_{sc}(\rho)$ is the sum of the trapping field and ion cloud space charge potential energies, respectively and p is the radial distance from the trap axis. Poisson's equation ($\nabla^2\varphi_{sc}(\rho) = -qn(\rho)/\epsilon_0$) leads to a non-linear differential equation for n(ρ)

$$n'' + n'/\rho - (n')^2/n + n(n_0 - n)/(n_0\lambda_D^2) = 0$$

where $n_0 = 2\epsilon_0 m\omega^2/q^2$ is the pseudocharge or saturation density for ions in the trap. The Debye length $\lambda_D^2 = iii,'lkP/(110q2) = k_BT/(2m\omega^2)$ is a measure of the penetration length of the time averaged trapping fields into the ion cloud interior. This equation is numerically solved (subject to $2\pi\int\rho n(\rho)d\rho = N/l$.) via Runge-Kutta methods to give. density profiles as shown in Figure 5. The 62 kHz trap secular frequency leads to a saturation density of 34,840 ions per mm³ which at S00 K ion temperature gives a Debye length 0.26 mm. l'mill $4\pi n_0 a^3/3 = 1$ we estimate an inter-ion spacing a = 19 μm at saturation density. The density profile determines the [eta] second order shift of the trapped ions as discussed in Appendix 1.

Ion Orbits

After the density equation has been solved the total potential seen by an ion is computed from $\Phi_{total}(\rho) = k_BT\cdot\ln(n(0)/n(\rho))$. An orbit in this 2-dimensional central force has two constants of motion [9], the angular momentum l_z around the z axis and the total energy in the (ρ,θ) plane E_{trans}, i.e., the kinetic plus potential energies. Following the procedures described in appendix 2 an initial position and velocity are generated consistent with the radial density profile for a set linear density N/1, and the

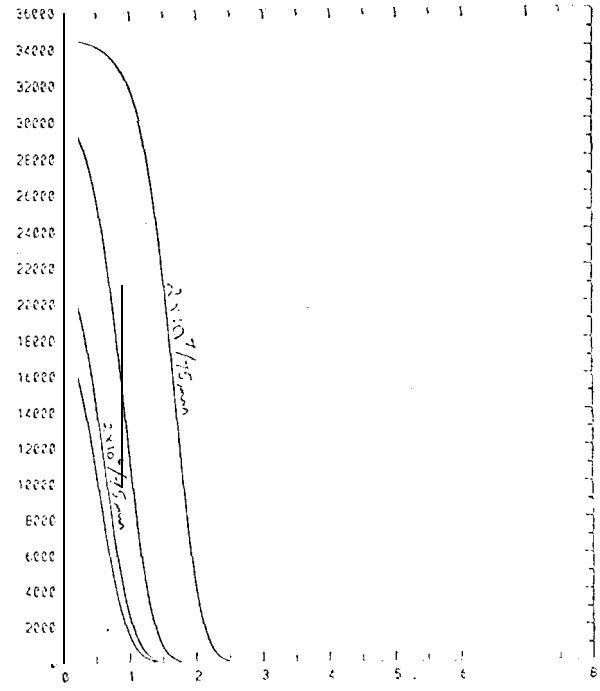

Figure S: Calculated ion density profiles for 500 K ion temperature at 62 kHz trap secular frequency. The highest density shown is $2x10^7$ ions in 75 mm length.

Maxwell-Boltzmann velocity distribution at temperature '1'. l_z and E_{trans} are computed at Ibis initial point and the radial turning points of the orbit are found by solving $E_{trans} - \Phi_{total}(\rho) - l_z^2/2m\rho^2 = O$. The orbits are integrated to tile radial turning points 10 find the angular turning points [9]

$$d\rho = (2(E_{trans} - \Phi_{total}(\rho) - l_z^2/2m\rho^2)/m)^{1/2}dt$$

$$d\Theta = (1/111\rho^2)dt.$$

Since the orbits are invariant under reflection about the turning points [9] the complete trajectory is generated by a number of successive reflections. The motion of an ion along the z-axis of the trap is assumed to be a uniform velocity (generated from the velocity distribution as described in Appendix 2) back and forth between the trap ends. For each initial condition a trajectory of duration ≈ 4msec is generated, A time scale common to all the trajectories is generated so that the autocorrelation function at each time step τ_n is averaged cover the 4,000 to 10,()(1() trajectories typically employed, 'Ibis function is then Fourier transformed to give the power spectral density seen by the ensemble of moving atoms.

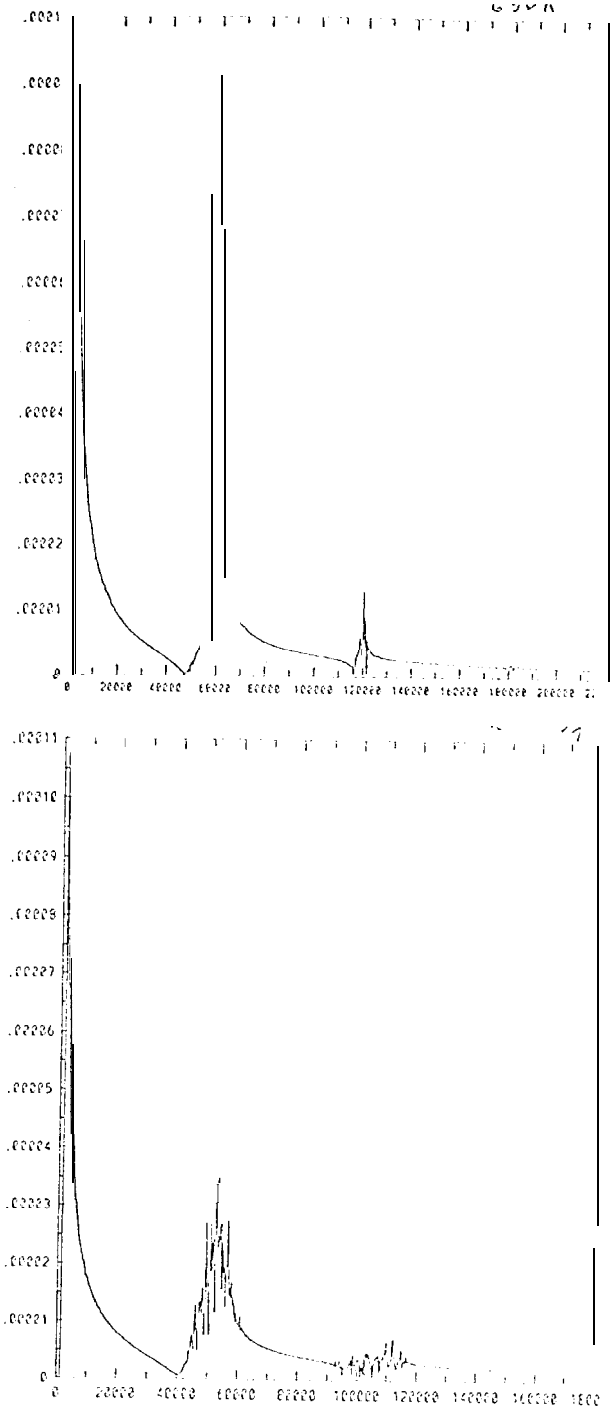

Figure 6: Simulated sideband structure for transverse propagation of 40.5 GHz radiation across ion cloud. The upper curve corresponds to 650 K with $5x10^5$ ions in 75 mm length. The lower curve at 650 K with $2,5x10^5$ ions in 75 mm has sidebands shifted in by 10 kHz from the 62 kHz trap secular frequency in agreement with the measured shift of Fig. 4(b).

Comparison with measured Sideband Frequency

Figure 6 shows the simulated sideband structure for a cloud of ions at 650 K of linear density $5x10^5$ ions per 75mm at 62, kHz trap secular frequency. Under these conditions the sidebands are sharp and are slightly displaced inward from the 62 kHz secular frequency. As the linear density is increased to about $2.5x10^6$/75mm the sidebands shift inward by about 10 kHz as shown in the measurement of Figure 4(b). The doppler frequency shift under these conditions is $-4.5x10^{-13}$ from thermal motion and $-4.3x10^{-13}$ from the micromotion generated by the trapping field. These are the approximate conditions for which the $^{199}Hg^+$ clock stability of $7x10^{-14}\tau^{-1/2}$ was obtained [4].

Conclusions

We have developed a spectroscopic method for measuring temperature, ion number and the resulting 2nd order Doppler shift of the 40.5 Ghz clock transition for $^{199}Hg^+$ ions in a linear ion trap. The ion cloud temperature is obtained from the Doppler broadened width of the 40.5 GHz Zeeman transition when the microwaves are propagated along the axis of the 1.1'1'. The ion number is then determined by modelling the frequency of the secular sidebands obtained when the 40.5 GHz radiation propagates across the ion cloud. In clock operation with $7x10^{-14}\tau^{-1/2}$ stability we have used this method to measure a $-8.8x10^{-13}$ frequency of fset due to 2nd order Doppler shift at 650 K and linear ion density $2.5x10^6$/75 mm.

Appendix 1: Total Second-Order Doppler Shift for fixed T and N/L

The resonance frequency, f_0, of an ion moving With total velocity \' will be shifted by Af from that of a stationary ion by $\Delta f/f_0 = -V^2/2c^2$. For an ion in an rf trap the velocity is the sum of a driven motion V_{micro} and a random thermal motion V_{th}. The micromotion velocity V_{micro} is determined by an ion's position in the trap whereas the magnitude and direction of V_{th} is uncorrelated with an ion's position. The average second order doppler shift for an ensemble of ions at temperature '1' is

$$-(V_{micro}+V_{th})^2/2c^2 = -(V_{micro}^2+V_{th}^2)/2c^2$$

because the average over the product $V_{micro} \cdot V_{th}$ vanishes. The two Sources call thus be Computed separately. Since the average of V_{th}^2 over the velocity distribution

is $3k_BT/m$, the contribution from the thermal motion is $-3k_BT/2mc^2$.

The contribution from the micro-motion is the average of V_{micro}^2 over the density distribution $n(\rho)$ as determined numerically from eq (l). The time averaged micro-motion grows with radial distance ρ, $V_{micro}^2 = \omega^2 \cdot \rho^2$ [10] so that

$$\bar{V}_{micro}^2 = \int n(\rho)\rho\omega^2\rho^2 d\rho / \int n(\rho)\rho d\rho.$$

In the limit of large λ_D, the solution to eq. (1) is $n(\rho) = n(0)\exp(-\rho^2/4\lambda_D^2)$ and the 2nd doppler from trap field generated ion motion is $-k_BT/mc^2$. This is 2/3 of the thermal contribution and stems from the fact that rf or ponderomotive forces provide the trapping in 2 of the 3 spatial dimensions. By contrast, when λ_D is very small compared to the ion cloud radius, the solution to eq. (1) is $n(\rho) = n_0$ out to the cloud radius $R_c = ((N/L)/n_0\pi)^{1/2}$. In this limit, the trap field induced 2nd order doppler shift is $-(q^2/8\pi\epsilon_0 mc^2)N/L$.

Appendix 2: Selection of Initial Positions and Velocities

The selection of the six initial position and velocity coordinates for an ion ensemble at temperature T with density distribution $n(\rho)$ is at the heart of the averaging procedure Used to compute the autocorrelation function. We follow the technique outlined in references [11,12] and will illustrate selection of the initial radial position coordinate. We compute the probability distribution for an ion's radial position from the. computed density profile $n(\rho)$. The number of ions found between ρ and $\rho + d\rho$ is $2\pi n(\rho)\rho d\rho$ so that the probability distribution for radial position $p(\rho)$ is

$$p(\rho) = n(\rho)\rho / \left(\int_0^\infty n(\rho)\rho d\rho\right).$$

A random number, ξ, is selected in the interval (0,1) with the. corresponding radial position ρ_ξ selected so that $\xi = \int_0^{\rho_\xi} p(\rho)d\rho$. The selection frequency of the radial position p is then in agreement with the distribution $p(\rho)$. All six of the initial values are chosen in this manner, the magnitude of the ion velocity from the Maxwell-Boltzmann distribution at temperature T, the. angle of the ion velocity along the trap longitudinal direction (z-axis) from $\Theta_\xi = \cos^{-1}(1-2\xi)$, and so forth. For each of the six initial values an independent random number ξ is chosen so tl~al.the.rc. is no correlation. A representative histogram of initial velocity components along the z direction generated from the speed and direction sampling is shown in Figure A(1) for an ion temperature of S00 K.

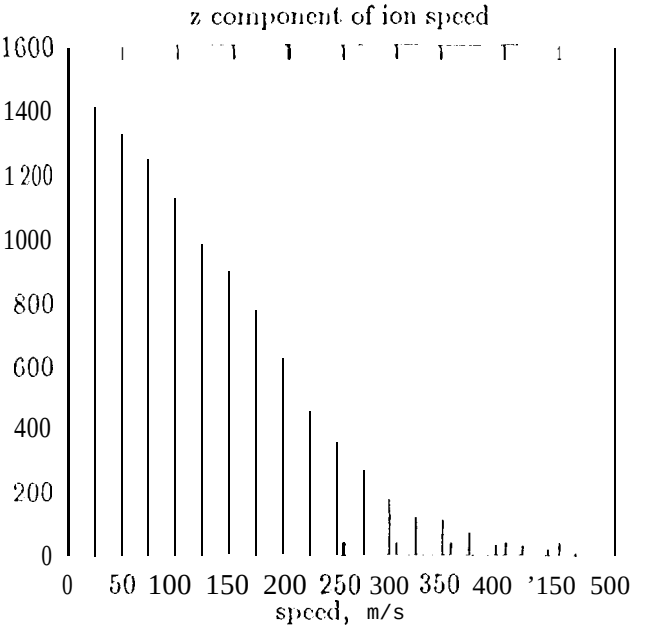

Figure A(1): The generated distribution of the z component of ion velocities. 'his histogram is created from two independently generated distributions- the Maxwell distribution of ion speeds and the velocity direction angle distribution with respect to the. trap longitudinal axis.

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